DS 4400

Machine Learning and Data Mining I

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Outline

- Classification
- Linear classification
- Perceptron
 - Online and batch perceptron
- LDA
 - Generative models
- Logistic regression
 - Classification based on probability

Supervised learning

Problem Setting

- Set of possible instances ${\mathcal X}$
- Set of possible labels ${\mathcal Y}$
- Unknown target function $f: \mathcal{X} \to \mathcal{Y}$
- Set of function hypotheses $H = \{h \mid h : \mathcal{X} \to \mathcal{Y}\}$

Input: Training examples of unknown target function f

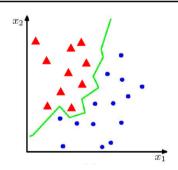
$$\{x_i, y_i\}$$
, for $i = 1, ..., n$

Output: Hypothesis $\hat{f} \in H$ that best approximates f

$$\hat{f}(x_i) \approx y_i$$

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Classification



Binary or discrete

• Suppose we are given a training set of N observations

$$\{x_1, ..., x_N\}$$
 and $\{y_1, ..., y_N\}, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$

• Classification problem is to estimate f(x) from this data such that

$$f(x_i) = y_i$$

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Example 1

Classifying spam email



GOOGLE LOTTERY INTERNATIONAL INTERNATIONAL PROMOTION / PRIZE AWARD . (WE ENCOURAGE GLOBALZATION) FROM: THE LOTTERY COORDINATOR, GOOGLE B.V. 44 9459 PE. RESULTS FOR CATEGORY "A" DRAWS

Congratulations to you as we bring to your notice, the results of the First Ca inform you that your email address have emerged a winner of One Million (1,1 money of I'wo Million (2,000,000 00) Euro shared among the 2 winners in this email addresses of individuals and companies from Africa, America, Asia, At CONGRATULATIONS!

Your fund is now deposited with the paying Bank. In your best interest to avo award strictly from public notice until the process of transferring your claims NOTE: to file for your claim, please contact the claim department below on e

Content-related features

- · Use of certain words
- · Word frequencies
- Language
- Sentence



Structural features

- Sender IP address
- IP blacklist
- DNS information
- Email server
- URL links (non-matching)

Binary classification: SPAM or HAM

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Example 2

Handwritten Digit Recognition















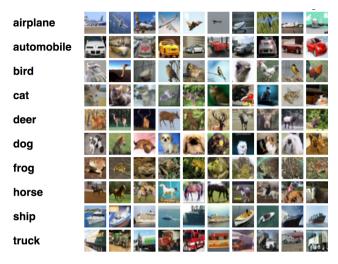






Example 3

Image classification



Multi-class classification

Supervised Learning Process Training Learning Pre-**Feature** Data processing extraction model Labeled Normalization Feature Classification (Typically) Standardization Selection Regression **Testing** New Learning **Predictions** model data Malicious Unlabeled Risk score Benign Classification Regression

History of Perceptrons

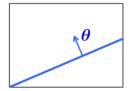
- They were popularised by Frank Rosenblatt in the early 1960's.
 - They appeared to have a very powerful learning algorithm.
 - Lots of grand claims were made for what they could learn to do.
- In 1969, Minsky and Papert published a book called "Perceptrons" that analysed what they could do and showed their limitations.
 - Many people thought these limitations applied to all neural network models.
- The perceptron learning procedure is still widely used today for tasks with enormous feature vectors that contain many millions of features.

They are the basic building blocks for Deep Neural Networks

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Linear classifiers

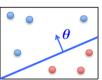
- A hyperplane partitions space into 2 half-spaces
 - Defined by the normal vector $~oldsymbol{ heta} \in \mathbb{R}^{~ extsf{d+1}}$
 - heta is orthogonal to any vector lying on the hyperplane



- Assumed to pass through the origin
 - This is because we incorporated bias term $\, heta_0\,$ into it by $\,x_0=1\,$
- Consider classification with +1, -1 labels ...

Linear classifiers

• Linear classifiers: represent decision boundary by hyperplane



$$h(\boldsymbol{x}) = \operatorname{sign}(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}) \text{ where } \operatorname{sign}(z) = \left\{ \begin{array}{cc} 1 & \text{if } z \geq 0 \\ -1 & \text{if } z < 0 \end{array} \right.$$

- Note that:
$$\boldsymbol{\theta}^\intercal x > 0 \implies y = +1$$
 $\boldsymbol{\theta}^\intercal x < 0 \implies y = -1$

All the points x on the hyperplane satisfy: $\theta^T x = 0$

Example: Spam

- Imagine 3 features (spam is "positive" class):
 - 1. free (number of occurrences of "free")
 - 2. money (occurrences of "money")
 - 3. BIAS (intercept, always has value 1)

$$\sum_{i=0}^{d} x_i \theta_i$$

"free money"

	л		
BIAS	:	1	
free	:	1	
money	:	1	

$$(1)(-3) + (1)(4) + (1)(2) + \dots$$

$$\sum_{i} x_{i} \theta_{i} > 0 \Rightarrow SPAM!!!$$

The Perceptron

$$h(x) = \operatorname{sign}(\theta^{\mathsf{T}} x)$$
 where $\operatorname{sign}(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ -1 & \text{if } z < 0 \end{cases}$

• The perceptron uses the following update rule each time it receives a new training instance (x_i, y_i)

$$\theta_j \leftarrow \theta_j - \frac{1}{2} (h_{\theta}(x_i) - y_i) x_{ij}$$
either 2 or -2

- If the prediction matches the label, make no change
- Otherwise, adjust θ

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The Perceptron

• The perceptron uses the following update rule each time it receives a new training instance (x_i, y_i)

$$\theta_j \leftarrow \theta_j - \frac{1}{2} (h_{\theta}(x_i) - y_i) x_{ij}$$
either 2 or -2

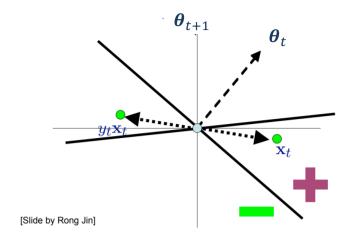
• Re-write as

$$\theta_j \leftarrow \theta_j + y_i x_{ij}$$

(only upon misclassification)

Perceptron Rule: If x_i is misclassified, do $\theta \leftarrow \theta + y_i x_i$

Geometric interpretation



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Online Perceptron

```
Let \theta \leftarrow [0,0,...,0]
Repeat:
Receive training example (x_i,y_i)
If y_i\theta^Tx_i \leq 0 // prediction is incorrect \theta \leftarrow \theta + y_i \ x_i
```

Online learning – the learning mode where the model update is performed each time a single observation is received

Batch learning – the learning mode where the model update is performed after observing the entire training set

Batch Perceptron

```
Given training data \begin{cases} x_i, y_i \end{cases}_{i=1}^n

Let \theta \leftarrow [0, 0, \dots, 0]

Repeat:

Let \Delta \leftarrow [0, 0, \dots, 0]

for i = 1 \dots n, do

if y_i \theta^T x_i \leq 0 // prediction for i<sup>th</sup> instance is incorrect

\Delta \leftarrow \Delta + y_i x_i

\Delta \leftarrow \Delta / n // compute average update

\theta \leftarrow \theta + \Delta

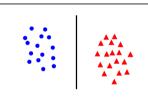
Until \|\Delta\|_2 < \epsilon
```

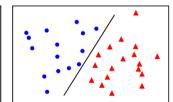
Guaranteed to find separating hyperplane if data is linearly separable

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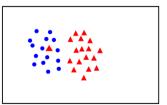
Linear separability

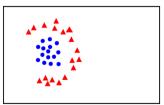
linearly separable





not linearly separable

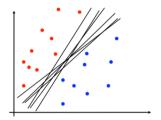




• For linearly separable data, can prove bounds on perceptron error (depends on how well separated the data is)

Perceptron Limitations

- Is dependent on starting point
- It could take many steps for convergence
- Perceptron can overfit
 - Move the decision boundary for every example



Which of this is optimal?

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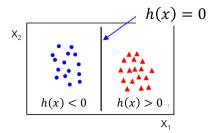
Improving the Perceptron

- The Perceptron produces many heta's during training
- The standard Perceptron simply uses the final heta at test time
 - This may sometimes not be a good idea!
 - Some other θ may be correct on 1,000 consecutive examples, but one mistake ruins it!
- Idea: Use a combination of multiple perceptrons
 - (i.e., neural networks!)
- Idea: Use the intermediate θ 's
 - **Voted Perceptron**: vote on predictions of the intermediate θ 's
 - Averaged Perceptron: average the intermediate θ 's

Linear classifiers

A linear classifier has the form

$$h_{\theta}(x) = f(\theta^T x)$$



- Properties
 - $(\theta_0, \theta_1, ..., \theta_d)$ = model parameters
 - Perceptron is a special case with f = sign
- Pros
 - Very compact model (size d)
 - Perceptron is fast
- Cons
 - Does not work for data that is not linearly separable





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LDA

- Classify to one of k classes
- Logistic regression computes directly
 - -P[Y=1|X=x]
 - Assume sigmoid function
- LDA uses Bayes Theorem to estimate it

$$-P[Y = k | X = x] = \frac{P[X = x | Y = k]P[Y=k]}{P[X=x]}$$

- Let $\pi_k = P[Y = k]$ be the prior probability of class k and $f_k(x) = P[X = x | Y = k]$

LDA

$$\Pr(Y = k | X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}.$$

Assume $f_k(x)$ is Gaussian! Unidimensional case (d=1)

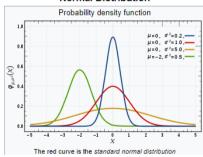
$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

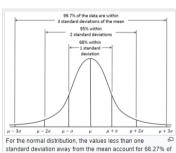
$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} (x - \mu_k)^2\right)}{\sum_{l=1}^K \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} (x - \mu_l)^2\right)}.$$

Assumption: $\sigma_1 = ... \sigma_k = \sigma$

Gaussian Distribution

Normal Distribution





the set; while two standard deviations from the mean account for 95.45%; and three standard deviations account for 99.73%

Notation	$\mathcal{N}(\mu, \sigma^2)$
Parameters	$\mu \in \mathbb{R}$ = mean (location)
	$\sigma^2>0$ = variance (squared scale)
Support	$x \in \mathbb{R}$
PDF	$\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(s-\mu)^2}{2\sigma^2}}$

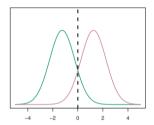
LDA decision boundary

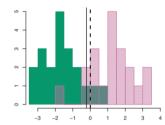
Pick class k to maximize

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

Example: k = 2, $\pi_1 = \pi_2$

Classify as class 1 if $x > \frac{\mu_1 + \mu_2}{2\sigma}$





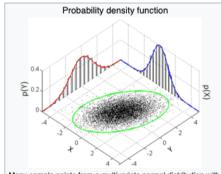
True decision boundary

Estimated decision boundary

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Multi-Variate Normal

Multivariate normal



Many sample points from a multivariate normal distribution with $\mu = \left[\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \right] \text{ and } \Sigma = \left[\begin{smallmatrix} 1 & 3/5 \\ 3/5 & 2 \end{smallmatrix} \right], \text{ shown along with the 3-sigma ellipse, the two marginal distributions, and the two 1-d histograms.}$

$$\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \, \boldsymbol{\Sigma}),$$

with k-dimensional mean vector

$$oldsymbol{\mu} = \mathrm{E}[\mathbf{X}] = [\mathrm{E}[X_1], \mathrm{E}[X_2], \ldots, \mathrm{E}[X_k]]^\mathrm{T},$$

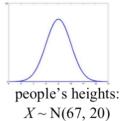
and k imes k covariance matrix

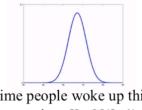
$$\Sigma_{i,j} =: \mathrm{E}[(X_i - \mu_i)(X_j - \mu_j)] = \mathrm{Cov}[X_i, X_j]$$

$$\mathbf{\Sigma} =: \mathbb{E}[(\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})^{\mathrm{T}}] = [\operatorname{Cov}[X_i, X_j]; 1 \leq i, j \leq k].$$

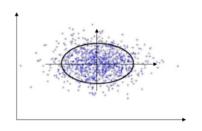
$$f_k(x) = \frac{1}{(2\pi)^{p/2} |\boldsymbol{\Sigma}_k|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \boldsymbol{\Sigma}_k^{-1}(x-\mu_k)}.$$

Example: Independent variables





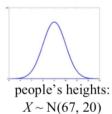
time people woke up this morning: $Y \sim N(9, 1)$

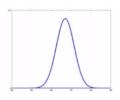


Co-variance matrix $\begin{bmatrix} 20 \\ 0 \end{bmatrix}$

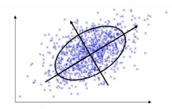
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Example: Correlated variables





People's weight $Y \approx N(177,40)$



Co-variance matrix l 5

Multi-variate LDA

$$\Pr(Y = k | X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^K \pi_l f_l(x)}.$$

Assume
$$\Sigma_k = \Sigma$$

$$\log \frac{\Pr(Y = k | X = x)}{\Pr(Y = l | X = x)z} = \log \frac{f_k(x)}{f_\ell(x)} + \log \frac{\pi_k}{\pi_\ell}$$
$$= \log \frac{\pi_k}{\pi_\ell} - \frac{1}{2} (\mu_k + \mu_\ell)^T \Sigma^{-1} (\mu_k - \mu_\ell)$$
$$+ x^T \Sigma^{-1} (\mu_k - \mu_\ell),$$

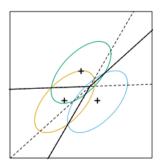
Linear decision boundary between classes k and l

Linear discriminant functions $\delta_k(x) = x^T \mathbf{\Sigma}^{-1} \mu_k - \frac{1}{2} \mu_k^T \mathbf{\Sigma}^{-1} \mu_k + \log \pi_k$

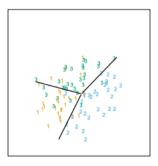
Given x, classify to class k: $argmax_k \delta_k(x)$

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Example 3 classes



3 Normal distributions with same co-variance, but different means



LDA decision boundary

LDA in practice

Given training data (x_i, y_i) , $i = 1, ..., n, y_i \in \{1, ..., K\}$

1. Estimate mean and variance

$$\hat{\mu}_{k} = \frac{1}{n_{k}} \sum_{i:y_{i}=k} x_{i}$$

$$\hat{\sigma}^{2} = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_{i}=k} (x_{i} - \hat{\mu}_{k})^{2}$$

2. Estimate prior

$$\hat{\pi}_k = n_k/n.$$

Given testing point x, predict k that maximizes:

$$\hat{\delta}_k(x) = x \cdot \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log(\hat{\pi}_k)$$

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Multi-variate LDA

Given training data (x_i, y_i) , $i = 1, ..., n, y_i \in \{1, ..., K\}$

1. Estimate mean and variance

- $\hat{\pi}_k = N_k/N$, where N_k is the number of class-k observations;
- μ̂_k = ∑_{a_i=k} x_i/N_k;
- $\hat{\Sigma} = \sum_{k=1}^{K} \sum_{g_i=k} (x_i \hat{\mu}_k) (x_i \hat{\mu}_k)^T / (N K).$
- 2. Estimate prior

Given testing point x, predict k that maximizes:

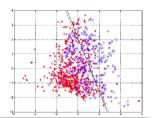
$$\delta_k(x) = x^T \mathbf{\Sigma}^{-1} \mu_k - \frac{1}{2} \mu_k^T \mathbf{\Sigma}^{-1} \mu_k + \log \pi_k$$

Classification based on Probability

- Instead of just predicting the class, give the probability of the instance being that class
 - i.e., learn $p(y \mid x)$
- · Comparison to perceptron:
 - Perceptron doesn't produce probability estimate
- · Recall that:

$$0 \le p(\text{event}) \le 1$$

 $p(\text{event}) + p(\neg \text{event}) = 1$



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Example

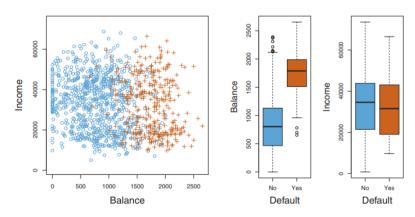


FIGURE 4.1. The Default data set. Left: The annual incomes and monthly credit card balances of a number of individuals. The individuals who defaulted on their credit card payments are shown in orange, and those who did not are shown in blue. Center: Boxplots of balance as a function of default status. Right: Boxplots of income as a function of default status.

Why not linear regression?

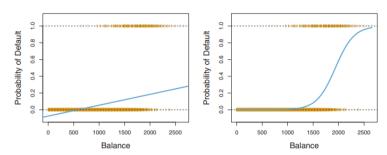


FIGURE 4.2. Classification using the Default data. Left: Estimated probability of default using linear regression. Some estimated probabilities are negative! The orange ticks indicate the 0/1 values coded for default (No or Yes). Right: Predicted probabilities of default using logistic regression. All probabilities lie between 0 and 1.

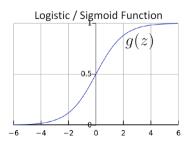
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Logistic regression

- Takes a probabilistic approach to learning discriminative functions (i.e., a classifier)
- $h_{m{ heta}}(m{x})$ should give $p(y=1\mid m{x}; m{ heta})$ Can't just use linear regression with a threshold
- · Logistic regression model:

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

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



Interpretation of Model Output

$$h_{\boldsymbol{\theta}}(\boldsymbol{x})$$
 = estimated $p(y=1 \mid \boldsymbol{x}; \boldsymbol{\theta})$

Example: Cancer diagnosis from tumor size

$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$$
 $h_{\theta}(\mathbf{x}) = 0.7$

→ Tell patient that 70% chance of tumor being malignant

Note that:
$$p(y = 0 \mid \boldsymbol{x}; \boldsymbol{\theta}) + p(y = 1 \mid \boldsymbol{x}; \boldsymbol{\theta}) = 1$$

Therefore,
$$p(y = 0 \mid \boldsymbol{x}; \boldsymbol{\theta}) = 1 - p(y = 1 \mid \boldsymbol{x}; \boldsymbol{\theta})$$

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LR is a Linear Classifier!

• Predict
$$y = 1$$
 if:

$$P[y = 1|x; \theta] > P[y = 0|x; \theta]$$

 $P[y = 1|x; \theta] > \frac{1}{1 + e^{-\theta^T x}} > \frac{1}{2}$

• Equivalent to:

$$\bullet e^{\theta_0 + \sum_{i=1}^d \theta_j x_j} > 1$$

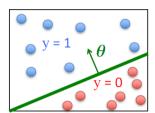
•
$$\theta_0 + \sum_{i=1}^d \theta_i x_i > 0$$

Logistic Regression is a linear classifier!

Logistic Regression

$$h_{m{ heta}}(m{x}) = g\left(m{ heta}^{\mathsf{T}}m{x}
ight)$$
 $g(z)$
$$g(z) = \frac{1}{1+e^{-z}}$$
 $g(z)$ $g(z)$

- Assume a threshold and...
 - Predict y = 1 if $h_{\theta}(x) \ge 0.5$
 - Predict y = 0 if $h_{\theta}(x) < 0.5$



Logistic Regression is a linear classifier!

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Logistic Regression

- Given $\left\{ \begin{array}{cccc} (x_1,y_1) &, & (x_2,y_2) &, \dots, & (x_N,y_N) \end{array} \right\}$ where $x_i \in R^d, y_i \in \{0,1\}$
- Model: $h_{m{ heta}}(m{x}) = g\left(m{ heta}^{\intercal}m{x}
 ight)$ $g(z) = \frac{1}{1+e^{-z}}$

Logistic Regression Objective

Can't just use squared loss as in linear regression:

$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} (h_{\theta}(x_i) - y_i)^2$$

- Using the logistic regression model

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

results in a non-convex optimization

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Maximum Likelihood Estimation (MLE)

Given training data $X = \{x_1, ..., x_N\}$ with labels $Y = \{y_1, ..., y_N\}$

What is the likelihood of training data for parameter θ ?

Define likelihood function

$$Max_{\theta} L(\theta) = P[Y|X; \theta]$$

Assumption: training points are independent

$$L(\theta) = \prod_{i=1}^{n} P[y_i|x_i;\theta]$$

General probabilistic method for classifier training

Log Likelihood

 Max likelihood is equivalent to maximizing log of likelihood

$$L(\theta) = \prod_{i=1}^{n} P[y_i | x_i, \theta]$$
$$\log L(\theta) = \sum_{i=1}^{n} \log P[y_i | x_i, \theta]$$

• They both have the same maximum $heta_{MLE}$

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MLE for Logistic Regression

$$p(y|x,\theta) = h_{\theta}(x)^{y} (1 - h_{\theta}(x))^{1-y}$$

$$\theta_{\text{MLE}} = \arg \max_{\theta} \sum_{i=1}^{n} \log p(y_{i}|,\theta)$$

$$= \arg \max_{\theta} \sum_{i=1}^{n} y_{i} \log h_{\theta}(x_{i}) + (1 - y_{i}) \log (1 - h_{\theta}(x_{i}))$$

· Substitute in model, and take negative to yield

Logistic regression objective:

$$\min_{\theta} J(\theta)$$

$$J(\theta) = -\sum_{i=1}^{n} y_i \log h_{\theta}(x_i) + (1 - y_i) \log (1 - h_{\theta}(x_i))$$

Objective for Logistic Regression

$$J(\theta) = -\sum_{i=1}^{n} y_{i} \log h_{\theta}(x_{i}) + (1 - y_{i}) \log (1 - h_{\theta}(x_{i}))$$

• Cost of a single instance:

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

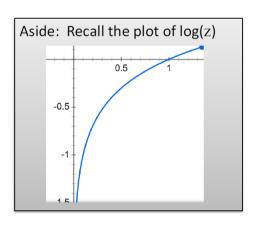
Can re-write objective function as

$$J(\boldsymbol{\theta}) = \sum_{i=1}^{n} \operatorname{cost} \left(h_{\boldsymbol{\theta}}(x_i), y_i \right)$$
Cross-entropy loss

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Intuition

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



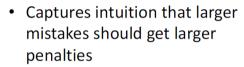
Intuition

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

If y = 1



• As
$$h_{\theta}(x) \to 0, \cos t \to \infty$$



$$-$$
 e.g., predict $\,h_{m{ heta}}(m{x})=0$, but ${
m y}$ = ${
m 1}$

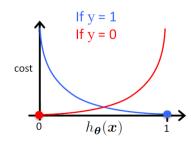
47

Intuition

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

If
$$y = 0$$

- Cost = 0 if prediction is correct
- As $(1 h_{\theta}(x)) \to 0$, $\cos t \to \infty$
- Captures intuition that larger mistakes should get larger penalties



If y = 1

 $h_{\boldsymbol{\theta}}(\boldsymbol{x})$

cost

Acknowledgements

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 - Andrew Ng
 - Eric Eaton
 - David Sontag
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