Gaussian and Linear Discriminant Analysis; Multiclass Classification

Professor Ameet Talwalkar

Outline

Announcements

- Homework 2: due on Wednesday

Outline

Logistic classification

Setup for two classes

- Input: $\boldsymbol{x} \in \mathbb{R}^D$
- Output: $y \in \{0, 1\}$
- Training data: $\mathcal{D} = \{(\boldsymbol{x}_n, y_n), n = 1, 2, \ldots, N\}$
- Model of *conditional distribution*

$$p(y = 1|\boldsymbol{x}; b, \boldsymbol{w}) = \sigma[g(\boldsymbol{x})]$$

where

$$g(\boldsymbol{x}) = b + \sum_d w_d x_d = b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$$

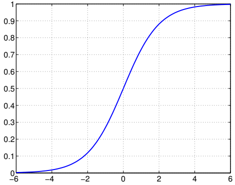
Why the sigmoid function?

What does it look like?

$$\sigma(a) = \frac{1}{1 + e^{-a}}$$

where

$$a = b + \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}$$



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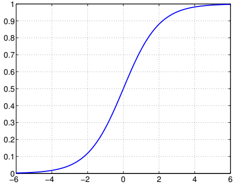

Properties

- Bounded between 0 and 1 $\leftarrow$ thus, interpretable as probability
- Monotonically increasing thus, usable to derive classification rules
  - $\sigma(a) > 0.5$, positive (classify as '1')
  - $\sigma(a) < 0.5$, negative (classify as '0')
  - $\sigma(a) = 0.5$, undecidable
- Nice computational properties Derivative is in a simple form

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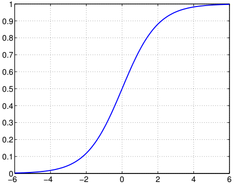

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Linear or nonlinear classifier?

Linear or nonlinear?

$\sigma(a)$ **is nonlinear**, however, the decision boundary is determined by

$$\sigma(a) = 0.5 \Rightarrow a = 0 \Rightarrow g(\boldsymbol{x}) = b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} = 0$$

which is a *linear* function in $\boldsymbol{x}$

We often call b the offset term.

Likelihood function

Probability of a single training sample $(\boldsymbol{x}_n, y_n)$

$$p(y_n|\boldsymbol{x}_n; b; \boldsymbol{w}) = \begin{cases} \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) & \text{if} \quad y_n = 1 \\ 1 - \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) & \text{otherwise} \end{cases}$$

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Compact expression, exploring that y_n is either 1 or 0

$$p(y_n|\boldsymbol{x}_n; b; \boldsymbol{w}) = \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)^{y_n}[1 - \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)]^{1-y_n}$$

Maximum likelihood estimation

Cross-entropy error (negative log-likelihood)

$$\mathcal{E}(b, \boldsymbol{w}) = -\sum_n \{y_n \log \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)]\}$$

Numerical optimization

- Gradient descent: simple, scalable to large-scale problems
- Newton method: fast but not scalable

Numerical optimization

Gradient descent

- Choose a proper step size $\eta > 0$
- Iteratively update the parameters following the negative gradient to minimize the error function

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \sum_n \left\{ \sigma(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) - y_n \right\} \boldsymbol{x}_n$$

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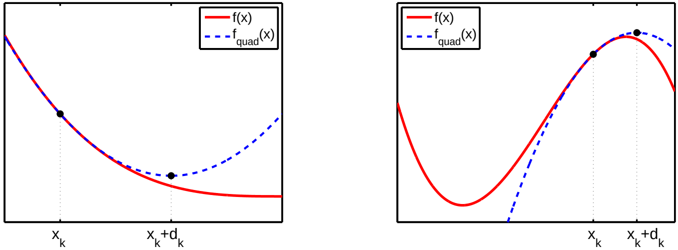
Remarks

- Gradient is direction of steepest ascent.
- The step size needs to be chosen carefully to ensure convergence.
- The step size can be adaptive (i.e. varying from iteration to iteration).
- Variant called *stochastic* gradient descent (later this quarter).

Intuition for Newton's method

Approximate the true function with an easy-to-solve optimization problem



In particular, we can approximate the cross-entropy error function around $\boldsymbol{w}^{(t)}$ by a quadratic function (its second order Taylor expansion), and then minimize this quadratic function

Update Rules

Gradient descent

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \sum_n \left\{ \sigma(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) - y_n \right\} \boldsymbol{x}_n$$

Newton method

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - {\boldsymbol{H}^{(t)}}^{-1} \nabla \mathcal{E}(\boldsymbol{w}^{(t)})$$

Contrast gradient descent and Newton's method

Similar

- Both are iterative procedures.

Different

- Newton's method requires second-order derivatives (less scalable, but faster convergence)
- Newton's method does not have the magic η to be set

Outline

Naive Bayes and logistic regression: two different modelling paradigms

Consider spam classification problem

- First Strategy:
  - Use training set to find a decision boundary in the feature space that separates spam and non-spam emails
  - Given a test point, predict its label based on which side of the boundary it is on.

Naive Bayes and logistic regression: two different modelling paradigms

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- Second Strategy:
  - Look at spam emails and build a model of what they look like. Similarly, build a model of what non-spam emails look like.
  - To classify a new email, match it against both the spam and non-spam models to see which is the better fit.

Naive Bayes and logistic regression: two different modelling paradigms

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First strategy is discriminative (e.g., logistic regression)
Second strategy is generative (e.g., naive bayes)

Generative vs Discriminative

Discriminative

- Requires only specifying a model for the conditional distribution $p(y|x)$, and thus, maximizes the *conditional* likelihood $\sum_n \log p(y_n|\boldsymbol{x}_n)$.
- Models that try to learn mappings directly from feature space to the labels are also discriminative, e.g., perceptron, SVMs (covered later)

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Generative

- Aims to model the joint probability $p(x, y)$ and thus maximize the *joint* likelihood $\sum_n \log p(\boldsymbol{x}_n, y_n)$.
- The generative models we'll cover do so by modeling $p(x|y)$ and $p(y)$

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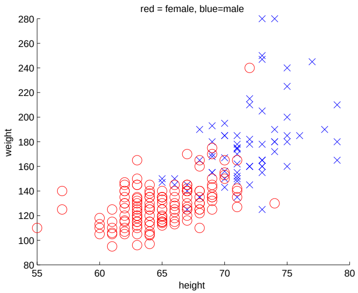
- The generative models we'll cover do so by modeling $p(x|y)$ and $p(y)$
- Let's look at two more examples: Gaussian (or Quadratic) Discriminative Analysis and Linear Discriminative Analysis

Determining sex based on measurements

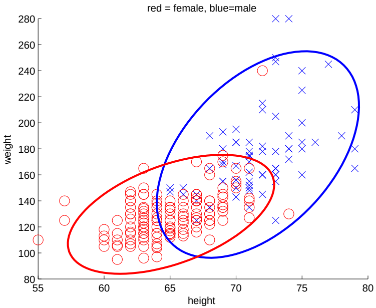


Generative approach

Model joint distribution of ($x =$ (height, weight), $y =$sex)

our data

Sex	Height	Weight
1	$6'$	175
0	$5'2"$	120
1	$5'6"$	140
1	$6'2"$	240
0	$5.7"$	130
$\cdots$	$\cdots$	$\cdots$

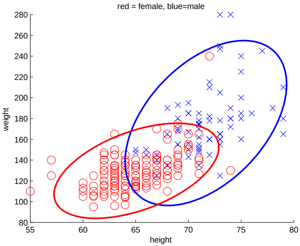


Intuition: we will model how heights vary (according to a Gaussian) in each sub-population (male and female).

Model of the joint distribution (1D)

$$p(x, y) = p(y)p(x|y)$$

$$= \begin{cases} p_0 \frac{1}{\sqrt{2\pi}\sigma_0} e^{-\frac{(x-\mu_0)^2}{2\sigma_0^2}} & \text{if } y = 0 \\ p_1 \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x-\mu_1)^2}{2\sigma_1^2}} & \text{if } y = 1 \end{cases}$$



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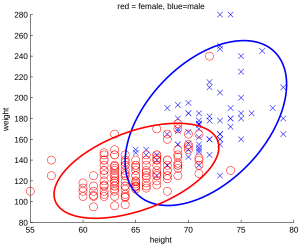

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What are the parameters to learn?

Parameter estimation

Log Likelihood of training data $\mathcal{D} = \{(x_n, y_n)\}_{n=1}^{N}$ with $y_n \in \{0, 1\}$

$$\log P(\mathcal{D}) = \sum_n \log p(x_n, y_n)$$

$$= \sum_{n:y_n=0} \log\left(p_0 \frac{1}{\sqrt{2\pi}\sigma_0} e^{-\frac{(x_n-\mu_0)^2}{2\sigma_0^2}}\right)$$

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- For Naive Bayes we assume $\boldsymbol{\Sigma}_i^*$ is diagonal

Decision boundary

As before, the Bayes optimal one under the assumed joint distribution depends on

$$p(y = 1|x) \geq p(y = 0|x)$$

which is equivalent to

$$p(x|y = 1)p(y = 1) \geq p(x|y = 0)p(y = 0)$$

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Namely,

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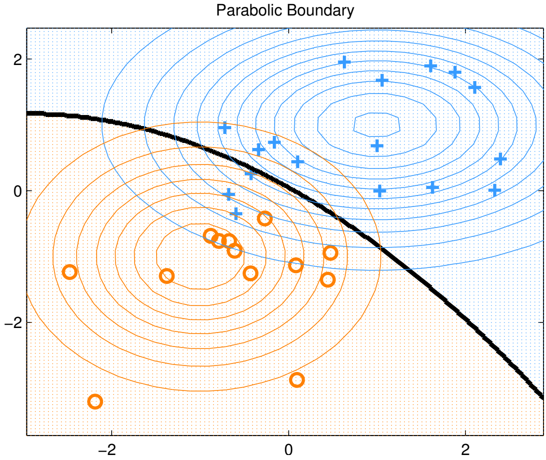
$\Rightarrow ax^2 + bx + c \geq 0 \qquad \leftarrow$ the decision boundary not *linear*!

Example of nonlinear decision boundary



Note: the boundary is characterized by a quadratic function, giving rise to the shape of a parabolic curve.

A special case: what if we assume the two Gaussians have the same variance?

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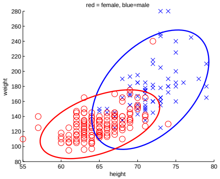
Note: equal variances across two different categories could be a very strong assumption.



For example, from the plot, it does seem that the *male* population has slightly bigger variance (i.e., bigger ellipse) than the *female* population. So the assumption might not be applicable.

Mini-summary

Gaussian discriminant analysis

- A generative approach, assuming the data modeled by

$$p(x, y) = p(y)p(x|y)$$

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- Parameters (of Gaussian distributions) estimated by max likelihood
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  - In general, nonlinear functions of x (*quadratic discriminant analysis*)
  - Linear under various assumptions about Gaussian covariance matrices
    - ★ *Single arbitrary* matrix (*linear discriminant analysis*)
    - ★ *Multiple diagonal* matrices (*Gaussian Naive Bayes (GNB)*)
    - ★ *Single diagonal* matrix (GNB in HW2 Problem 1)

So what is the discriminative counterpart?

Intuition

The decision boundary in Gaussian discriminant analysis is

$$ax^2 + bx + c = 0$$

Let us model the conditional distribution analogously

$$p(y|x) = \sigma[ax^2 + bx + c] = \frac{1}{1 + e^{-(ax^2+bx+c)}}$$

Or, even simpler, going after the decision boundary of linear discriminant analysis

$$p(y|x) = \sigma[bx + c]$$

Both look very similar to logistic regression — i.e. we focus on writing down the *conditional* probability, *not* the joint probability.

Does this change how we estimate the parameters?

First change: a smaller number of parameters to estimate

Models only parameterized by a, b and c. There are no prior probabilities (p_0, p_1) or Gaussian distribution parameters (μ_0, μ_1, σ_0 and σ_1).

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Second change: maximize the conditional likelihood $p(y|x)$

$$
\begin{aligned}
(a^*, b^*, c^*) = \arg\min -\sum_n \{ & y_n \log \sigma(ax_n^2 + bx_n + c) && (1)\\
& + (1 - y_n) \log[1 - \sigma(ax_n^2 + bx_n + c)]\} && (2)
\end{aligned}
$$

No closed form solutions!

How easy for our Gaussian discriminant analysis?

Example

$$p_1 = \frac{\#\text{ of training samples in class 1}}{\#\text{ of training samples}} \tag{3}$$

$$\mu_1 = \frac{\sum_{n:y_n=1} x_n}{\#\text{ of training samples in class 1}} \tag{4}$$

$$\sigma_1^2 = \frac{\sum_{n:y_n=1} (x_n - \mu_1)^2}{\#\text{ of training samples in class 1}} \tag{5}$$

Note: see textbook for detailed derivation (including generalization to higher dimensions and multiple classes)

Generative versus discriminative: which one to use?

There is no fixed rule

- Selecting which type of method to use is dataset/task specific
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- Selecting which type of method to use is dataset/task specific
- It depends on how well your modeling assumption fits the data
- For instance, as we show in HW2, when data follows a specific variant of the Gaussian Naive Bayes assumption, $p(y|x)$ necessarily follows a logistic function. However, the converse is not true.
  - Gaussian Naive Bayes makes a stronger assumption than logistic regression
  - When data follows this assumption, Gaussian Naive Bayes will likely yield a model that better fits the data
  - But logistic regression is more robust and less sensitive to incorrect modelling assumption

Outline

Setup

Predict multiple classes/outcomes: $C_1, C_2, \ldots, C_K$

- Weather prediction: sunny, cloudy, raining, etc
- Optical character recognition: 10 digits + 26 characters (lower and upper cases) + special characters, etc

Studied methods

- Nearest neighbor classifier
- Naive Bayes
- Gaussian discriminant analysis
- Logistic regression

Logistic regression for predicting multiple classes? Easy

The approach of "one versus the rest"

- For each class C_k, change the problem into binary classification
  1. Relabel training data with label C_k, into POSITIVE (or '1')
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  This step is often called *1-of-K* encoding. That is, only one is nonzero and everything else is zero.

  Example: for class C_2, data go through the following change

$$(\boldsymbol{x}_1, C_1) \rightarrow (\boldsymbol{x}_1, 0), (\boldsymbol{x}_2, C_3) \rightarrow (\boldsymbol{x}_2, 0), \ldots, (\boldsymbol{x}_n, C_2) \rightarrow (\boldsymbol{x}_n, 1), \ldots,$$

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- Train K binary classifiers using logistic regression to differentiate the two classes
- When predicting on $\boldsymbol{x}$, combine the outputs of all binary classifiers
  1. What if all the classifiers say NEGATIVE?
  2. What if multiple classifiers say POSITIVE?

Yet, another easy approach

The approach of "one versus one"

- For each *pair* of classes C_k and $C_{k'}$, change the problem into binary classification
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- Train $K(K-1)/2$ binary classifiers using logistic regression to differentiate the two classes
- When predicting on $\boldsymbol{x}$, combine the outputs of all binary classifiers
  There are $K(K-1)/2$ votes!

Contrast these two approaches

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Bad about both of them

Combining classifiers' outputs seem to be a bit tricky.

Any other good methods?

Multinomial logistic regression

Intuition: from the decision rule of our naive Bayes classifier

$$
\begin{aligned}
y^* &= \arg\max_k p(y = C_k|\boldsymbol{x}) = \arg\max_k \log p(\boldsymbol{x}|y = C_k)p(y = C_k) \\
&= \arg\max_k \log \pi_k + \sum_i z_i \log \theta_{ki} = \arg\max_k \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}
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Essentially, we are comparing

$$
\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x}, \boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x}, \cdots, \boldsymbol{w}_{\mathsf{K}}^{\mathrm{T}}\boldsymbol{x}
$$

with *one* for each category.

First try

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But we are close!
We can learn the K linear models jointly to ensure this property holds!

Definition of multinomial logistic regression

Model

For each class C_k, we have a parameter vector $\boldsymbol{w}_k$ and model the posterior probability as

$$p(C_k|\boldsymbol{x}) = \frac{e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}}}{\sum_{k'} e^{\boldsymbol{w}_{k'}^{\mathrm{T}}\boldsymbol{x}}} \qquad \leftarrow \qquad \text{This is called } \textit{softmax} \text{ function}$$

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Decision boundary: assign $\boldsymbol{x}$ with the label that is the maximum of posterior

$$\arg\max_k P(C_k|\boldsymbol{x}) \rightarrow \arg\max_k \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}$$

How does the softmax function behave?

Suppose we have

$$\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x} = 100, \boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x} = 50, \boldsymbol{w}_3^{\mathrm{T}}\boldsymbol{x} = -20$$

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We would pick the *winning* class label 1.

Softmax translates these scores into well-formed conditional probababilities

$$p(y = 1|\boldsymbol{x}) = \frac{e^{100}}{e^{100} + e^{50} + e^{-20}} < 1$$

- preserves relative ordering of scores
- maps scores to values between 0 and 1 that also sum to 1

Sanity check

Multinomial model reduce to binary logistic regression when $K = 2$

$$p(C_1|\boldsymbol{x}) = \frac{e^{\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x}}}{e^{\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x}} + e^{\boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x}}} = \frac{1}{1 + e^{-(\boldsymbol{w}_1 - \boldsymbol{w}_2)^{\mathrm{T}}\boldsymbol{x}}}$$
$$= \frac{1}{1 + e^{-\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}}}$$

Multinomial thus generalizes the (binary) logistic regression to deal with multiple classes.

Parameter estimation

Discriminative approach: maximize conditional likelihood

$$\log P(\mathcal{D}) = \sum_n \log P(y_n|\boldsymbol{x}_n)$$

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We will change y_n to $\boldsymbol{y}_n = [y_{n1}\ y_{n2}\ \cdots\ y_{nK}]^{\mathrm{T}}$, a K-dimensional vector using 1-of-K encoding.

$$y_{nk} = \begin{cases} 1 & \text{if } y_n = k \\ 0 & \text{otherwise} \end{cases}$$

Ex: if $y_n = 2$, then, $\boldsymbol{y}_n = [0\ 1\ 0\ 0\ \cdots\ 0]^{\mathrm{T}}$.

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$$\Rightarrow \sum_n \log P(y_n|\boldsymbol{x}_n) = \sum_n \log \prod_{k=1}^{K} P(C_k|\boldsymbol{x}_n)^{y_{nk}} = \sum_n \sum_k y_{nk} \log P(C_k|\boldsymbol{x}_n)$$

Cross-entropy error function

Definition: negative log likelihood

$$\mathcal{E}(\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_K) = -\sum_n \sum_k y_{nk} \log P(C_k | \boldsymbol{x}_n)$$

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Properties

- Convex, therefore unique global optimum
- Optimization requires numerical procedures, analogous to those used for binary logistic regression