CSCI567 Machine Learning (Fall 2016)

Dr. Yan Liu

yanliu.cs@usc.edu

September 21, 2016

Outline

1. Multiclass classification
   - Multinomial logistic regression
2. Generative versus discriminative

Setup

Suppose we need to 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

Contrast these two approaches

Pros and cons of each approach

- *one versus the rest*: only needs to train K classifiers. Make a *huge* difference if you have a lot of *classes* to go through.
  Can you think of a good application example where there are a lot of classes?
- *one versus one*: only needs to train a smaller subset of data (only those labeled with those two classes would be involved). Make a *huge* difference if you have a lot of *data* to go through.

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

$$y^* = \arg\max_c p(y = c|\boldsymbol{x}) = \arg\max_c \log p(\boldsymbol{x}|y = c)p(y = c) \quad (1)$$

$$= \arg\max_c \log \pi_c + \sum_k z_k \log \theta_{ck} = \arg\max_c \boldsymbol{w}_c^{\mathrm{T}} \boldsymbol{x} \quad (2)$$

Essentially, we are comparing

$$\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x}, \boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x}, \cdots, \boldsymbol{w}_{\mathsf{C}}^{\mathrm{T}}\boldsymbol{x} \quad (3)$$

with *one* for each category.

First try

So, can we define the following conditional model?

$$p(y = c|\boldsymbol{x}) = \sigma[\boldsymbol{w}_c^{\mathrm{T}}\boldsymbol{x}]$$

This would *not* work at least for the reason

$$\sum_c p(y = c|\boldsymbol{x}) = \sum_c \sigma[\boldsymbol{w}_c^{\mathrm{T}}\boldsymbol{x}] \neq 1$$

as each the summand can be any number (independently) between 0 and 1. *But we are close*

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

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

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

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

Note: the notation is changed to denote the classes as C_k instead of just c

Why the name softmax?

Suppose we have

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

we could have picked the *winning* class label 1 with certainty according to our classification rule.

Softness comes in when we compute the probability of selecting that

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

despite it being the largest among the 3 $p(y = 1|\boldsymbol{x}) > p(y = 2|\boldsymbol{x})$ and $p(y = 1|\boldsymbol{x}) > p(y = 3|\boldsymbol{x})$. Thus the name *softmax*

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

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

Parameter estimation

Discriminative approach: maximize conditional likelihood

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

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, $\boldsymbol{y}_n = [0\ 1\ 0\ 0\ \cdots\ 0]^{\mathrm{T}}$.

Parameter estimation

Discriminative approach: maximize conditional likelihood

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

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, $\boldsymbol{y}_n = [0\ 1\ 0\ 0\ \cdots\ 0]^{\mathrm{T}}$.

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

Cross-entropy error function

Definition:negated likelihood

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

Cross-entropy error function

Definition:negated likelihood

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

Properties

- Convex, therefore unique global optimum
- Optimization requires numerical procedures, analogous to those used for binary logistic regression
  Large-scale implementation, in both the number of classes and the training examples, is non-trivial.

Outline

1. Multiclass classification
2. Generative versus discriminative
    - Contrast Naive Bayes and logistic regression
    - Another example: Gaussian discriminant analysis

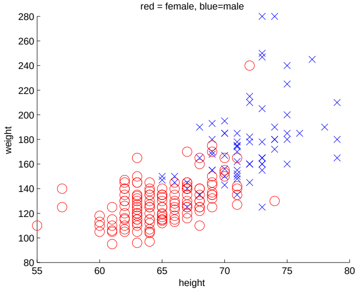
Naive Bayes and logistic regression: two different modeling paradigms

- Setup of the learning problem
  Suppose the training data is from an *unknown* joint probabilistic model $p(\boldsymbol{x}, y)$
- Differences in *assuming* models for the data
  - the generative approach requires we specify the model for the joint distribution (such as Naive Bayes), and thus, maximize the *joint* likelihood $\sum_n \log p(\boldsymbol{x}_n, y_n)$
  - the discriminative approach (discriminative) requires only specifying a model for the conditional distribution (such as logistic regression), and thus, maximize the *conditional* likelihood $\sum_n \log p(y_n|\boldsymbol{x}_n)$

Naive Bayes and logistic regression: two different modeling paradigms

- Setup of the learning problem
  Suppose the training data is from an *unknown* joint probabilistic model $p(\boldsymbol{x}, y)$
- Differences in *assuming* models for the data
  - the generative approach requires we specify the model for the joint distribution (such as Naive Bayes), and thus, maximize the *joint* likelihood $\sum_n \log p(\boldsymbol{x}_n, y_n)$
  - the discriminative approach (discriminative) requires only specifying a model for the conditional distribution (such as logistic regression), and thus, maximize the *conditional* likelihood $\sum_n \log p(y_n|\boldsymbol{x}_n)$
- Differences in computation
  - Sometimes, modeling by discriminative approach is easier
  - Sometimes, parameter estimation by generative approach is easier

Determining sex (man or woman) based on measurements

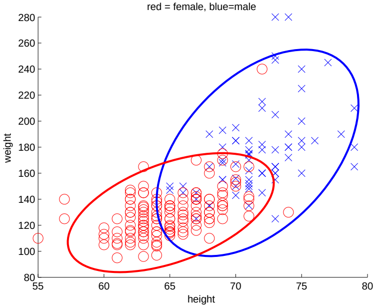


Generative approach

Propose a model of the joint distribution of (x = height, y =sex)

our data

Sex	Height
1	$6'$
2	$5'2$”
1	$5'6$”
1	$6'2$”
2	5.7”
...	...



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

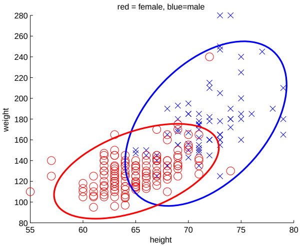
Note: This is similar to Naive Bayes for detecting spam emails.

Model of the joint distribution

$$p(x, y) = p(y)p(x|y) \tag{4}$$

$$= \begin{cases} p_1 \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x-\mu_1)^2}{2\sigma_1^2}} & \text{if } y = 1 \\ p_2 \frac{1}{\sqrt{2\pi}\sigma_2} e^{-\frac{(x-\mu_2)^2}{2\sigma_2^2}} & \text{if } y = 2 \end{cases} \tag{5}$$

where $p_1 + p_2 = 1$ represents two *prior* probabilities that x is given the label 1 or 2 respectively. $p(x|y)$ is called *class distributions*, which we have assumed to be Gaussians.



Parameter estimation

Likelihood of the training data $\mathcal{D} = \{(x_n, y_n)\}_{n=1}^{N}$ with $y_n \in \{1, 2\}$

$$\begin{aligned}
\log P(\mathcal{D}) &= \sum_n \log p(x_n, y_n) \\
&= \sum_{n:y_n=1} \log \left(p_1 \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x_n-\mu_1)^2}{2\sigma_1^2}} \right) \\
&+ \sum_{n:y_n=2} \log \left(p_2 \frac{1}{\sqrt{2\pi}\sigma_2} e^{-\frac{(x_n-\mu_2)^2}{2\sigma_2^2}} \right)
\end{aligned}$$

Parameter estimation

Likelihood of the training data $\mathcal{D} = \{(x_n, y_n)\}_{n=1}^N$ with $y_n \in \{1, 2\}$

$$\begin{aligned}\log P(\mathcal{D}) &= \sum_n \log p(x_n, y_n) \\ &= \sum_{n:y_n=1} \log \left(p_1 \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x_n-\mu_1)^2}{2\sigma_1^2}} \right) \\ &+ \sum_{n:y_n=2} \log \left(p_2 \frac{1}{\sqrt{2\pi}\sigma_2} e^{-\frac{(x_n-\mu_2)^2}{2\sigma_2^2}} \right)\end{aligned}$$

Maximize the likelihood function

$$(p_1^*, p_2^*, \mu_1^*, \mu_2^*, \sigma_1^*, \sigma_2^*) = \arg\max \log P(\mathcal{D})$$

Decision boundary

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

$$p(y = 1|x) \geq p(y = 2|x)$$

which is equivalent to

$$p(x|y = 1)p(y = 1) \geq p(x|y = 2)p(y = 2)$$

Decision boundary

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

$$p(y=1|x) \geq p(y=2|x)$$

which is equivalent to

$$p(x|y=1)p(y=1) \geq p(x|y=2)p(y=2)$$

Namely,

$$-\frac{(x-\mu_1)^2}{2\sigma_1^2} - \log\sqrt{2\pi}\sigma_1 + \log p_1 \geq -\frac{(x-\mu_2)^2}{2\sigma_2^2} - \log\sqrt{2\pi}\sigma_2 + \log p_2$$

Decision boundary

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

$$p(y = 1|x) \geq p(y = 2|x)$$

which is equivalent to

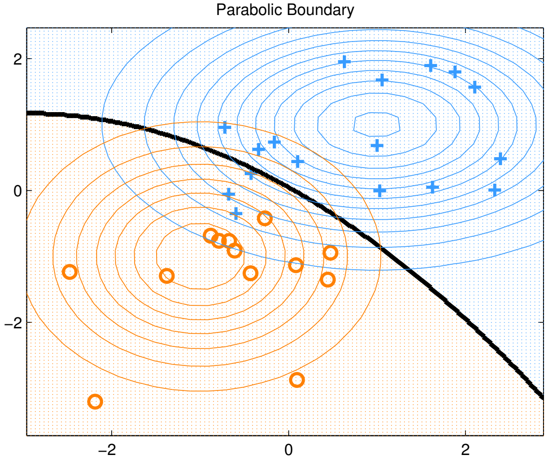
$$p(x|y = 1)p(y = 1) \geq p(x|y = 2)p(y = 2)$$

Namely,

$$- \frac{(x - \mu_1)^2}{2\sigma_1^2} - \log \sqrt{2\pi}\sigma_1 + \log p_1 \geq - \frac{(x - \mu_2)^2}{2\sigma_2^2} - \log \sqrt{2\pi}\sigma_2 + \log p_2$$

$\Rightarrow ax^2 + bx + c \geq 0$ $\leftarrow$ 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 parabolic curve.

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

We will get a linear decision boundary

$$-\frac{(x-\mu_1)^2}{2\sigma_1^2} - \log\sqrt{2\pi}\sigma_1 + \log p_1 \geq -\frac{(x-\mu_2)^2}{2\sigma_2^2} - \log\sqrt{2\pi}\sigma_2 + \log p_2$$

with $\sigma_1 = \sigma_2$, we have

$$bx + c \geq 0$$

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

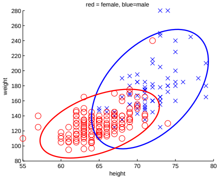
We will get a linear decision boundary

$$-\frac{(x-\mu_1)^2}{2\sigma_1^2} - \log\sqrt{2\pi}\sigma_1 + \log p_1 \geq -\frac{(x-\mu_2)^2}{2\sigma_2^2} - \log\sqrt{2\pi}\sigma_2 + \log p_2$$

with $\sigma_1 = \sigma_2$, we have

$$bx + c \geq 0$$

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 eclipse) than the *female* population. So the assumption might not be applicable.

Mini-summary

Gaussian discriminant analysis

- A generative approach, assuming the data modeled by

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

  where $p(x|y)$ is a Gaussian distribution.
- Parameters (of those Gaussian distributions) are estimated by maximizing the likelihood
  - Computationally, estimating those parameters are very easy — it amounts to computing sample mean vectors and covariance matrices
- Decision boundary
  - In general, nonlinear functions of x — in this case, we call the approach *quadratic discriminant analysis*
  - In the special case we assume equal variance of the Gaussian distributions, we get a linear decision boundary — we call the approach *linear discriminant analysis*

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

Our models are only parameterized by a, b and c. There is no prior probabilities (p_1, p_2) or Gaussian distribution parameters (μ_1, μ_2, σ_1 and σ_2).

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

$$(a^*, b^*, c^*) = \arg\min - \sum_n \{y_n \log \sigma(ax_n^2 + bx_n + c) \quad (6)$$

$$+ (1 - y_n) \log[1 - \sigma(ax_n^2 + bx_n + c)]\} \quad (7)$$

Computationally, much harder!

How easy for our Gaussian discriminant analysis?

Example

$$\hat{p}_1 = \frac{\#\text{ of training samples in class 1}}{\#\text{ of training samples}} \tag{8}$$

$$\hat{\mu}_1 = \frac{\sum_{n:y_n=1} x_n}{\#\text{ of training samples in class 1}} \tag{9}$$

$$\hat{\sigma}_1^2 = \frac{\sum_{n:y_n=1}(x_n - \mu_1)^2}{\#\text{ of training samples in class 1}} \tag{10}$$

Note: detailed derivation is in the books. They can be generalized rather easily to multi-variate distributions as well as 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
- It depends on how well your modeling assumption fits the data
- Recent trend: big data is always useful for both!
  - Apply very complex discriminative models, such as deep learning methods, for building classifiers
  - Apply very complex generative models, such as nonparametric Bayesian methods, for modeling data