

S&DS 265 / 565
Introductory Machine Learning








Classification (continued)

September 20

Upcoming items

- Assn 1 due on week from Thursday (midnight, 11:59pm)
- Submit *both* your `.ipynb` notebook and a printout as `.pdf` (save as HTML then print as pdf).
- Quiz 2 will be posted on Thursday
- As before, Quiz 2 will be available on Canvas for 24 hours starting at noon; you have 20 minutes to take the quiz once started
- Questions?

Updates to Calendar iml.ydata123.org

Week	Dates	Topics	Demos & Tutorials	Lecture Slides	Readings and Notes	Assignments & Exams
1	Sept 1	Course overview		Sept 1: Course overview		
2	Sept 6, 8	Python and background concepts	 Python elements  Covid trends	Sept 6: Python elements Sept 8: Pandas and linear regression	Data8 Chapters 3, 4, 5	Thu: Quiz 1
3	Sept 13, 15	Linear regression and classification	 Covid trends (revisited)  Classification examples	Sept 13: Regression concepts Sept 15: Classification	Notes on regression and classification	Thu:  Assn1 out
4	Sept 20, 22	Stochastic gradient descent	 SGD examples	Sept 20: Classification (continued) Sept 22: Stochastic gradient descent		Thu: Quiz 2
			 SGD examples			

Many parts of the notes are



Outline

- Logistic regression (continued)
- Iris example
- Generative vs. discriminative
- Gaussian discriminant analysis
- Regularization
- Example: Supernovae
- Next: Algorithms for fitting the models

Recall: Important concepts

Binary classifier h : function from \mathcal{X} to $\{0, 1\}$.

Linear if exists a function $H(x) = \beta_0 + \beta^T x$ such that $h(x) = 1$ if $H(x) > 0$; 0 otherwise.

$H(x)$ also called a *linear discriminant function*. Decision boundary:
set $\{x \in \mathbb{R}^d : H(x) = 0\}$

Recall: Important concepts

Classification risk, or *error rate*, of h :

$$R(h) = \mathbb{P}(Y \neq h(X))$$

and the *empirical classification error* or *training error* is

$$\hat{R}(h) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}(h(x_i) \neq y_i).$$

Optimal classification rule

The most accurate rule possible is called the *Bayes rule*.

The risk $R^* = R(h^*)$ of the Bayes rule is called the *Bayes risk*.

The Bayes decision rule

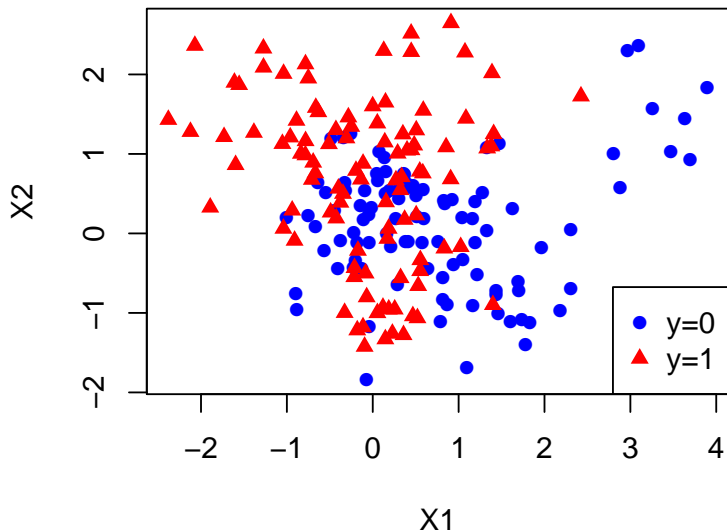
From Bayes' theorem

$$\mathbb{P}(Y = 1 | X = x) = \frac{p(x | Y = 1)\mathbb{P}(Y = 1)}{p(x | Y = 1)\mathbb{P}(Y = 1) + p(x | Y = 0)\mathbb{P}(Y = 0)}$$

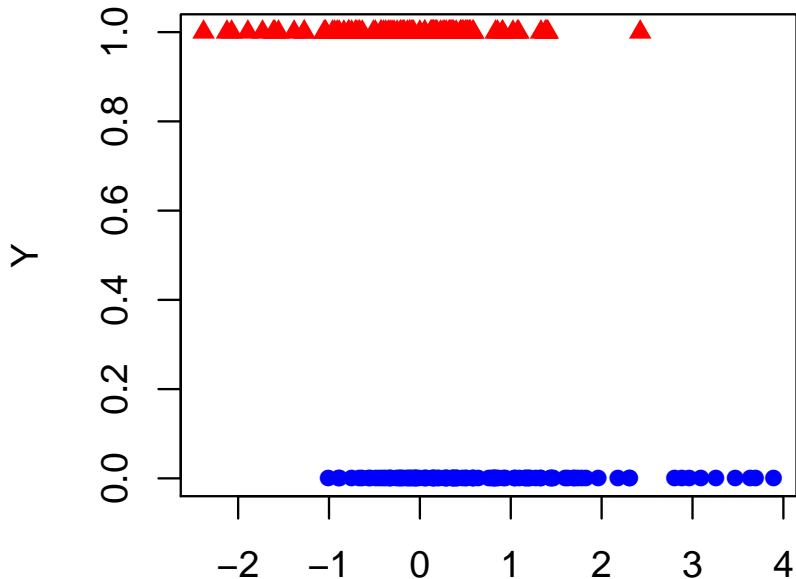
So,

$$h^*(x) = 1 \quad \text{is equivalent to} \quad \frac{p(x | Y = 1)}{p(x | Y = 0)} > \frac{\mathbb{P}(Y = 0)}{\mathbb{P}(Y = 1)}.$$

Simulated data: Large Bayes error



Simplification—one predictor: Large Bayes error



Logistic regression

Conditional probabilities of the class:

$$\mathbb{P}(Y = 1 \mid X = x) \equiv p(x)$$

$$\mathbb{P}(Y = 0 \mid X = x) = 1 - p(x)$$

Logistic regression

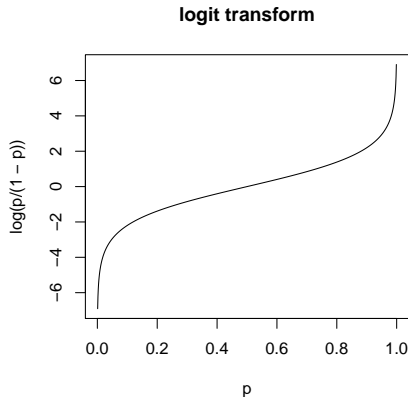
Conditional probabilities of the class:

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We model the relationship between $p(x)$ and x .

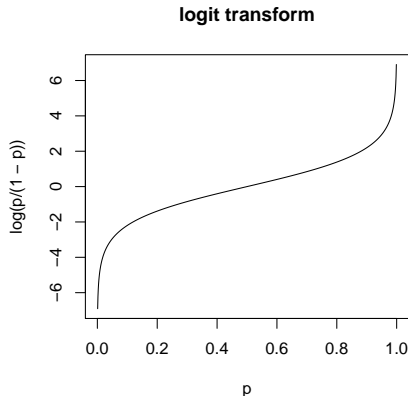
Logistic regression



The *logit* transform:

$$\text{logit}(p) = \log\left(\frac{p}{1-p}\right)$$

Logistic regression



The *logit* transform:

$$\text{logit}(p) = \log\left(\frac{p}{1-p}\right)$$

The logit transform

- is monotone
- maps the interval $[0, 1]$ to $(-\infty, \infty)$

Logistic regression

Logistic regression is a linear regression model of the log odds:

$$\text{logit}(p(x)) = \beta_0 + \beta_1 x$$

- p is a probability.
- $\frac{p}{1-p}$ is **odds**.
- $\text{logit}(p) = \log\left(\frac{p}{1-p}\right)$ is (natural) **log odds**.

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Equivalent formulation:

$$p(x) = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}} = \text{logistic}(x^T \beta) \equiv \text{softmax}(x^T \beta)$$

Extension to more than 2 classes

Multinomial logistic regression extends the logistic regression model to $K \geq 2$ classes.

$$\log \left(\frac{P(Y = k | X = x)}{P(Y = 0 | X = x)} \right) = x^T \beta_k, \quad k = 1, 2, \dots, K - 1$$

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$$P(Y = k | X = x) = \begin{cases} \frac{\exp(x^T \beta_k)}{1 + \sum_{l=1}^{K-1} \exp(x^T \beta_l)} & k = 1, 2, \dots, K - 1 \\ \frac{1}{1 + \sum_{l=1}^{K-1} \exp(x^T \beta_l)} & k = 0 \end{cases}$$

Loss function for 3 classes

We want to maximize the likelihood of the data, which is equivalent to minimizing the log-likelihood:

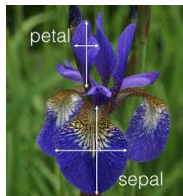
$$\begin{aligned} & - \sum_{i=1}^n \log P(Y = y_i | X = x_i) \\ & = \sum_{i=1}^n \left\{ \log(1 + e^{\beta_1^T x_i} + e^{\beta_2^T x_i}) - \beta_{y_i}^T x_i \right\} \end{aligned}$$

keeping in mind that β_0 is all zeros, by definition.

Fisher's iris classification



Iris setosa (Left), *Iris versicolor* (Middle), and *Iris virginica* (Right).



Examples in Jupyter notebook

Last time we worked through some examples in the demo Jupyter notebook. Please download `classification-examples.ipynb` and run the notebook to be sure you understand everything!

Regularization

Recall from last time: We can separate *setosa* from the two other species just on the basis of their petal length (or width).

This causes problems when we fit the model — the parameters get large so that the probabilities get very close to zero or one.

To address this problem, we *regularize* the parameters. This means we introduce a penalty term that prevents them from getting too large (in absolute value).

Regularization: Simplest setting

The least squares estimator:

$$\hat{\beta} = \arg \min_{\beta} (y - \beta)^2$$

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Solution: $\hat{\beta} = \frac{y}{1+\lambda}$.

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Now *penalize* β from getting too large:

$$\hat{\beta} = \arg \min_{\beta} (y - \beta)^2 + \lambda \beta^2$$

Solution: $\hat{\beta} = \frac{y}{1+\lambda}$. As λ gets large, $\hat{\beta}$ shrinks to zero.

Two flavors of classifiers

Generative models model both the input X and the output Y .

Discriminative models model only the output Y given X .

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Generative models model both the input X and the output Y .

Discriminative models model only the output Y given X .

Which do you think is better?

Generative models

We build a model of the inputs x and the outputs y

In the generative case we typically estimate the joint distribution by maximizing the *joint likelihood*: $p(x, y)$

Discriminative models

In the discriminative case we are concerned about the *conditional* distribution of the output given the input.

We will typically estimate by maximizing the *conditional likelihood*:

The form of the Bayes classification rule suggests we should use a generative model

$$m_{\theta}(x) \equiv \mathbb{P}(Y = 1 \mid X = x) = \frac{\pi_1 p_{\theta_1,1}(x)}{(1 - \pi_1) p_{\theta_0,0}(x) + \pi_1 p_{\theta_1,1}(x)}.$$

Given an estimator $(\hat{\theta}_n, \hat{\pi}_1)$, define classification rule

$$\hat{h}(x) = \mathbb{1}(m_{\hat{\theta}_n}(x) > 1/2).$$

where $\mathbb{1}$ is the “indicator function” which is 1 if its argument is true, and zero otherwise.

Gaussian discriminant analysis

- A type of generative model
- We model the inputs x using Gaussians
- Two flavors: Linear and Quadratic

Quadratic discriminant analysis

In the binary (two-class) case, we have two Gaussians:

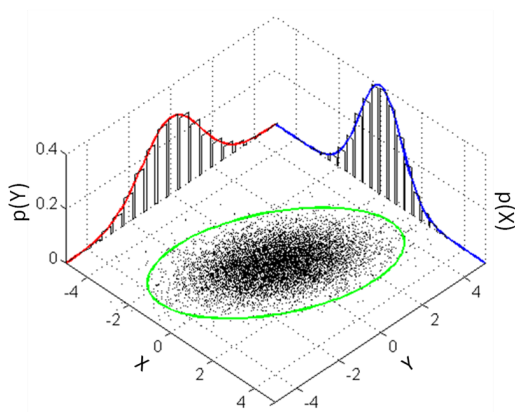
$$X \mid y = 1 \sim N(\mu_1, \Sigma_1)$$

$$X \mid y = 0 \sim N(\mu_0, \Sigma_0)$$

The decision boundary is a quadratic surface (algebra!)

Quadratic discriminant analysis

To estimate this we just separate the training data according to the two labels and estimate two separate Gaussians. Easy-peasy!



Think of Y here as another predictor variable, not the class label!

https://en.wikipedia.org/wiki/Multivariate_normal_distribution

Linear discriminant analysis

In the binary (two-class) case, we again have two Gaussians:

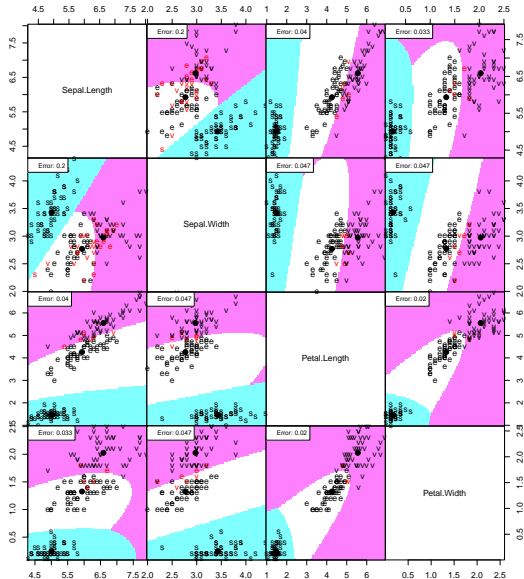
$$X \mid y = 1 \sim N(\mu_1, \Sigma)$$

$$X \mid y = 0 \sim N(\mu_0, \Sigma)$$

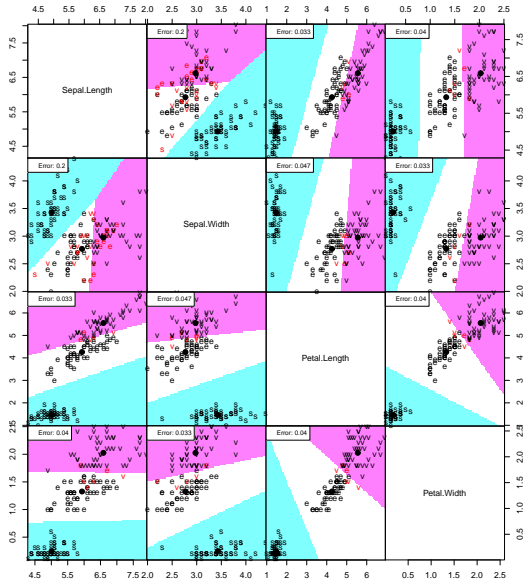
But now we use the same covariance matrix for each.

The decision boundary is now *linear*.

Quadratic discriminant analysis: Iris data



Linear discriminant analysis: Iris data



Logistic regression

Logistic regression is a discriminative model, because we don't have a model for the inputs X .

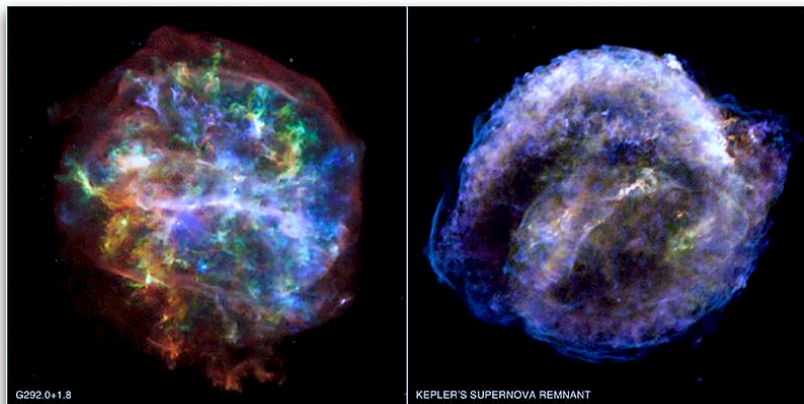
We only model the conditional probability $p(Y | X)$.

Logistic regression is the discriminative version of linear discriminative analysis (the latter is a generative model).

Supernovæ

- A *supernova* is an exploding star.
- Type Ia supernovae are very useful in astrophysics research. Have a characteristic *light curve*, same maximum brightness
- Since we know both the absolute and apparent (measured) brightness of a type Ia supernova, we can compute its distance.
- Astronomers also measure the *redshift* of the supernova, the speed at which the supernova is moving away from us
- The relationship between distance and redshift provides important information about the large scale structure of the universe.

Supernovae

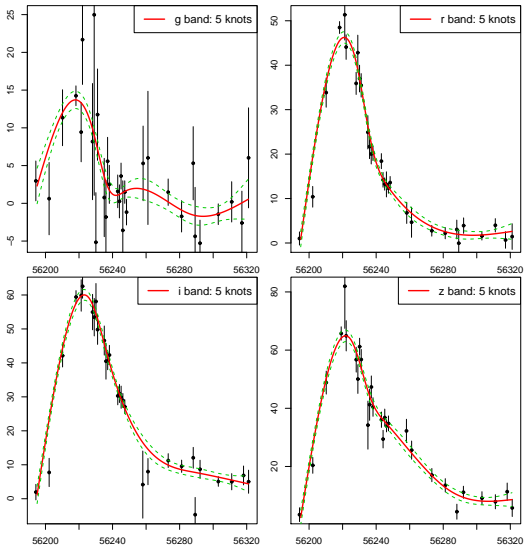


Two supernova remnants from the NASA's Chandra X-ray Observatory study. The right one is Type Ia. (Credit: NASA/CXC/UCSC/L. Lopez et al.)

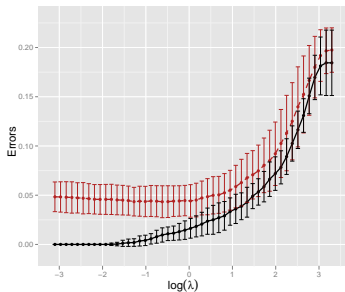
Supernovae

- Data are 20,000 real and simulated supernovae.
- For each supernova, there are a few noisy measurements of the flux (brightness) in four different filters — *g*-band (green), *r*-band (red), *i*-band (infrared) and *z*-band (blue).
- These noisy data are processed to fit a curve through the measurements in each band, the values along this curve are used as predictor variables

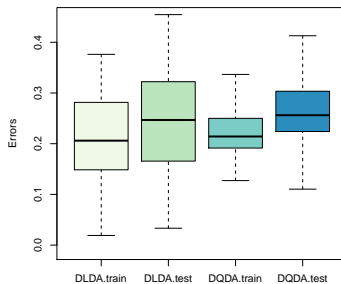
Supernovae



Supernovae – classification results



Logistic Regression



Discriminant Analysis

Fitting a logistic regression model

- We maximize conditional likelihood. There is no closed form.
- Need to iterate.
- Standard approach is equivalent to Newton's algorithm
 - ▶ Make a quadratic approximation
 - ▶ Do a weighted least squares regression
 - ▶ Repeat

We'll talk about a more scalable approach next time

Summary

- Classifiers come in two flavors: generative & discriminative
- Linear Gaussian discriminant analysis is a simple generative classifier
- Logistic regression is the discriminative version. Default method; no closed-form solution
- We regularize the parameters with a penalty β^2 that keeps them from being too big. *Shrinks* coefficients toward zero.