



S&DS 265 / 565
Introductory Machine Learning

Classification (continued)

September 19

Yale

Upcoming items

- Assn 1 due 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 next Thursday
- Questions?

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

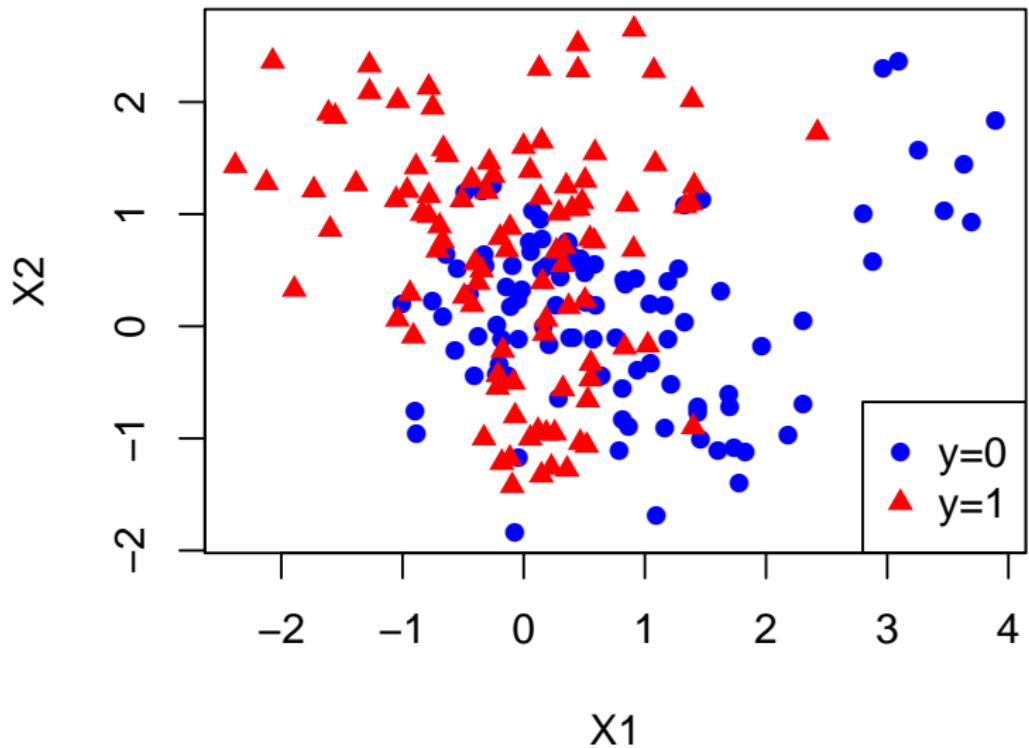
From Bayes' theorem

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

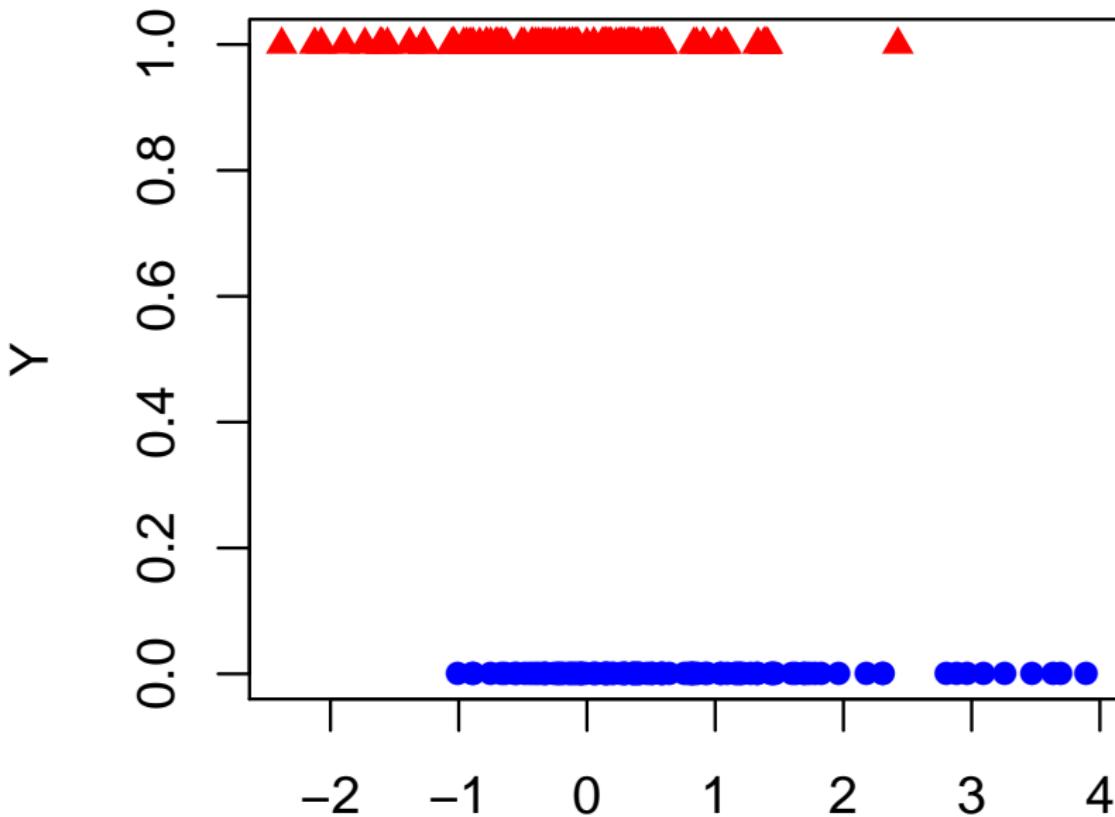
So,

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

Simulated data: Large Bayes error



Simplification—one predictor: Large Bayes error



Logistic regression

Conditional probabilities of the class:

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

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

Logistic regression

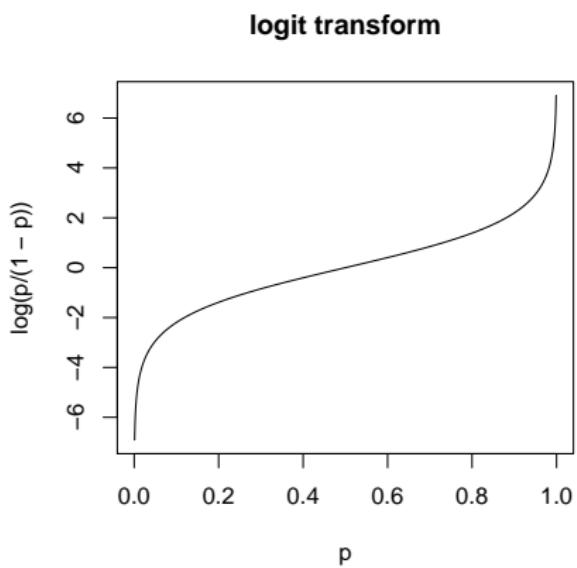
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We model the relationship between $p(x)$ and x .

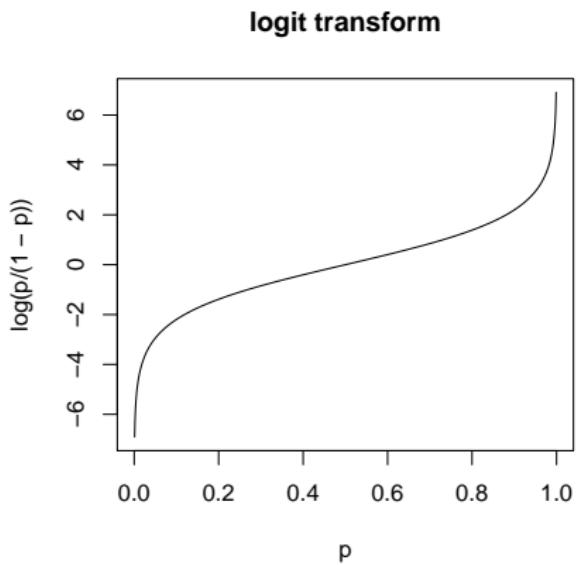
Logistic regression



The *logit* transform:

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

Logistic regression



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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:

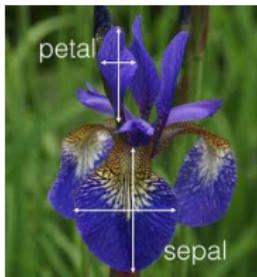
$$\begin{aligned} - \sum_{i=1}^n \log P(Y = y_i | X = x_i) \\ = \sum_{i=1}^n \left\{ \log(1 + e^{\beta_1^T x_i} + e^{\beta_2^T x_i}) - \beta_{y_i}^T x_i \right\} \end{aligned}$$

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

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

Two flavors of classifiers

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

Discriminative: model only the output Y given X .

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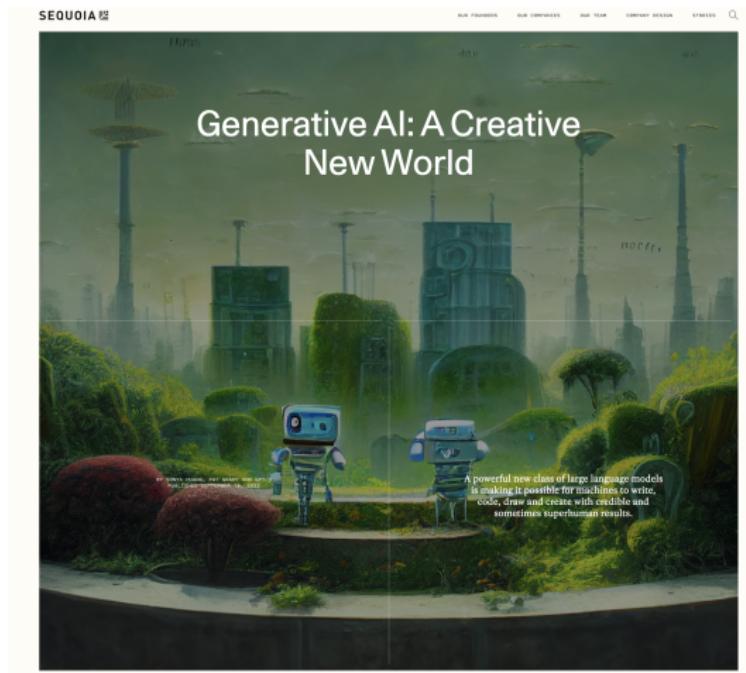
Which do you think is better?

Generative models

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

In the generative case we typically estimate the model by trying to maximize the *joint likelihood* $p(x, y)$ of the training data

Generative models



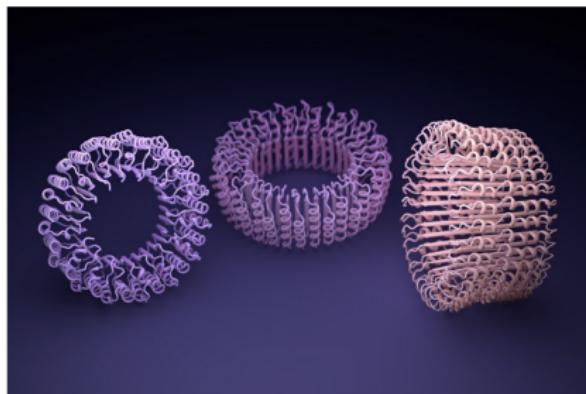
Generative models

NEWS | 15 September 2022

Scientists are using AI to dream up revolutionary new proteins

Huge advances in artificial intelligence mean researchers can design completely original molecules in seconds instead of months.

Ewen Callaway



Artificial-intelligence tools are helping to scientists to come up with proteins that are shaped unlike anything in nature. Credit: Ian C Haydon/UW Institute for Protein Design

Discriminative models

In the discriminative case we focus on the *conditional* distribution of the output given the input

We will typically estimate by maximizing the *conditional likelihood* of the training data

Bayes rule

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

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

But we can target the discriminant function directly

Gaussian discriminant analysis

- A type of generative model — *unfortunate terminology!*
- 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:

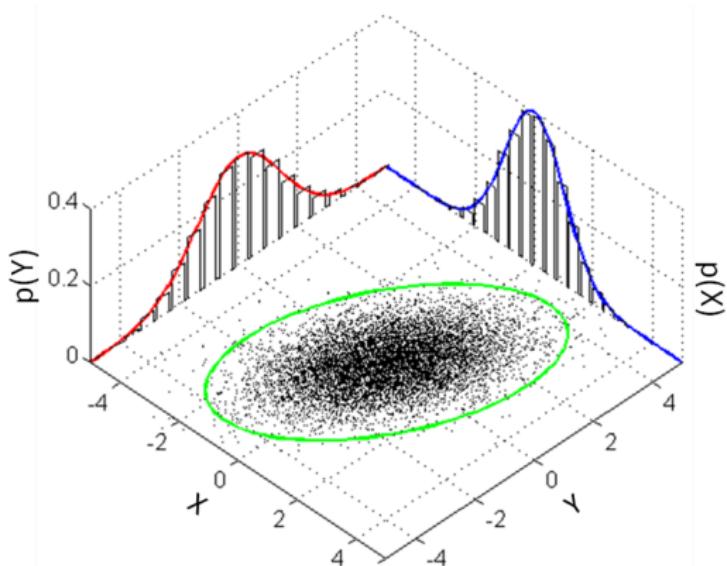
$$X \mid y = 1 \sim N(\mu_1, \Sigma_1)$$

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

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:

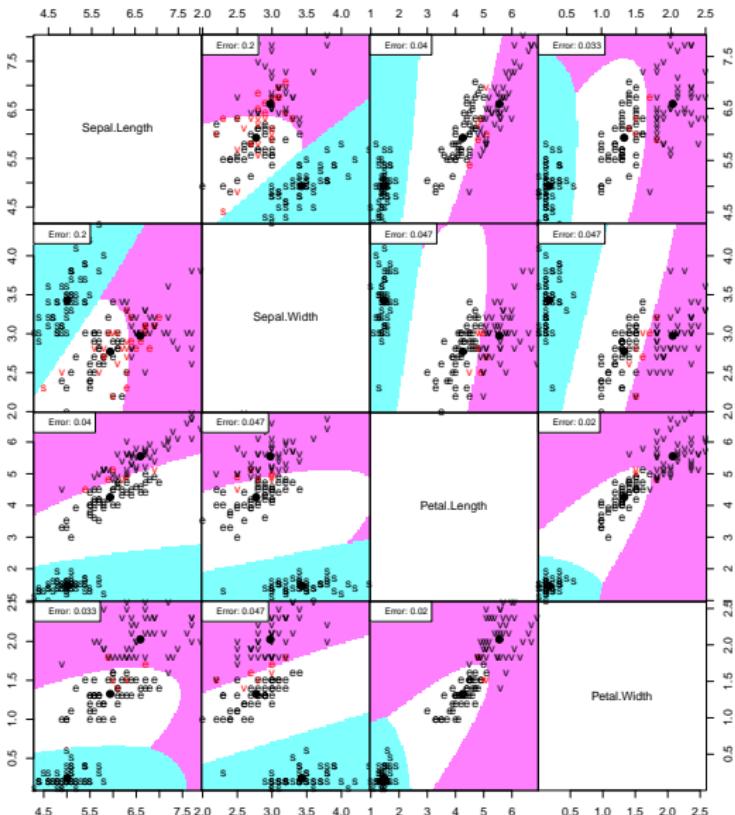
$$X | y = 1 \sim N(\mu_1, \Sigma)$$

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

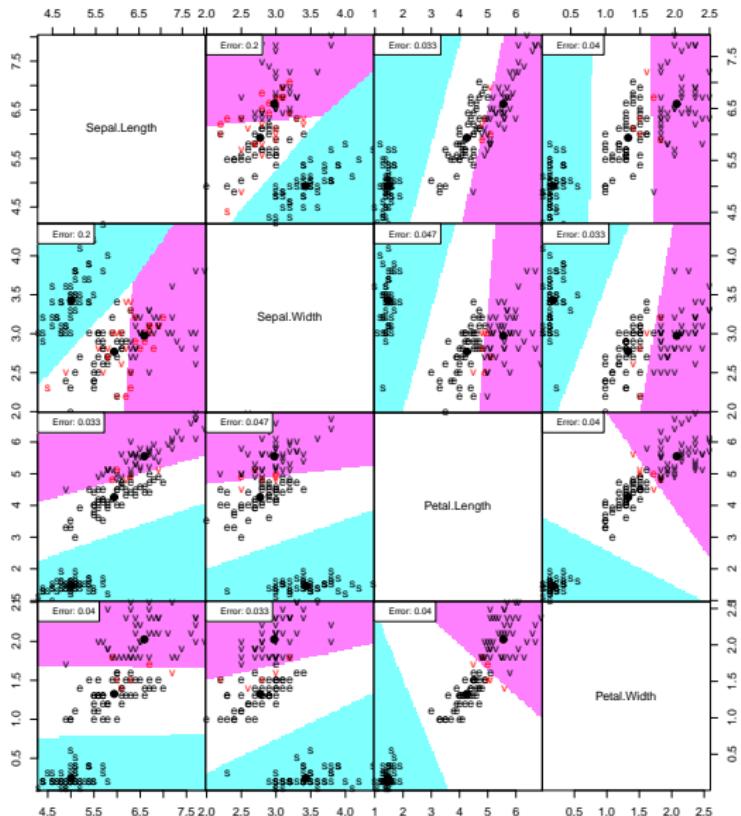
But now we use the *same covariance* matrix for each.

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 .

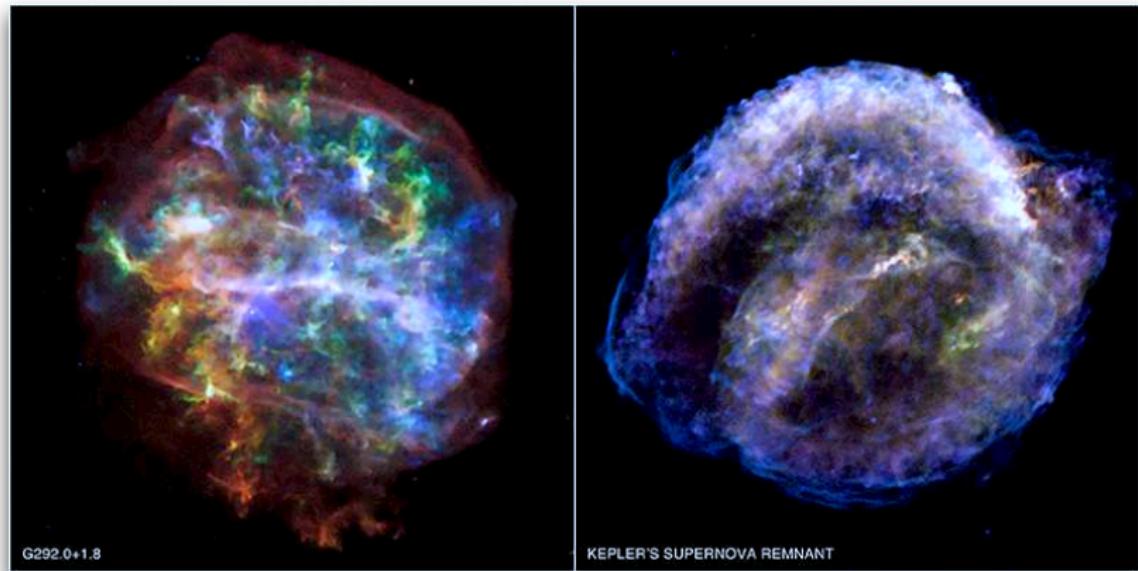
We only model the conditional probability $p(Y | X)$.

Logistic regression is the discriminative version of linear discriminant analysis (the latter is a generative model—unfortunate terminology!)

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

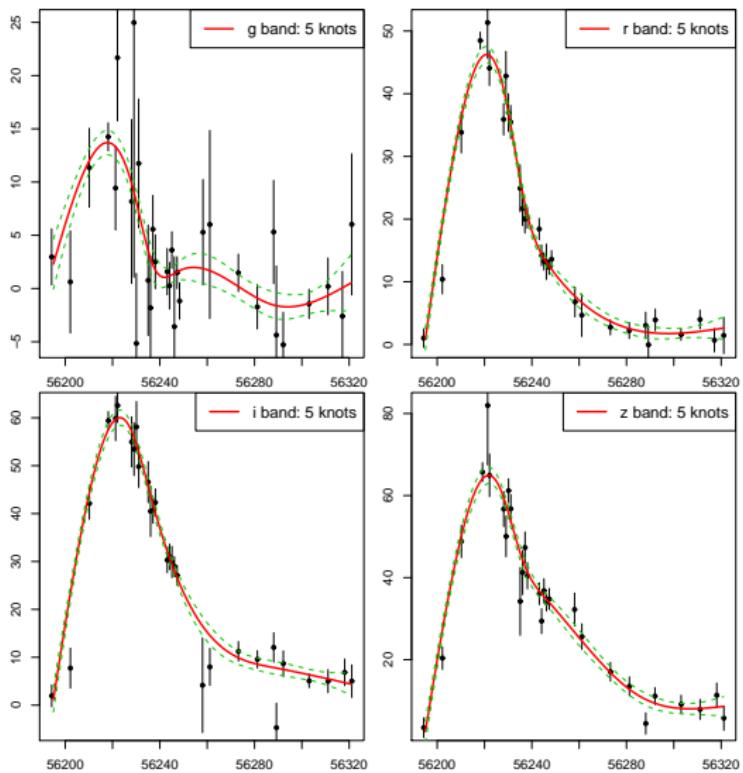


Two supernova remnants from the NASA's Chandra X-ray Observatory study. The right one is Type Ia. (Credit: NASA/CXC/UCSC/L. Lopez et al.)

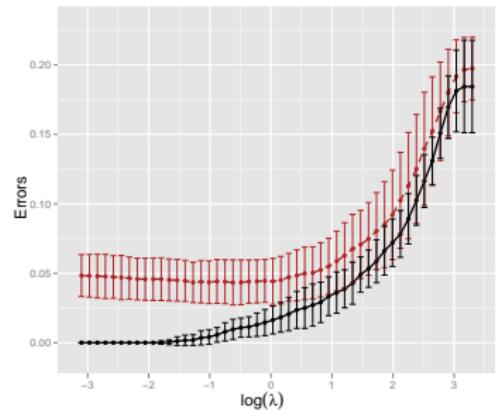
Supernovae

- 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

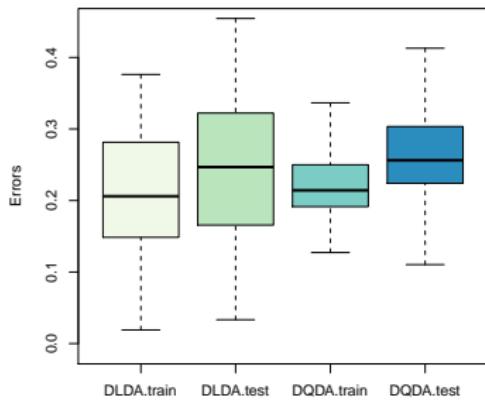
Supernovae



Supernovae – classification results



Logistic Regression



Discriminant Analysis

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.