Stat 406: Algorithms for classification and prediction

Lecture 1: Introduction

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Wed 4 January, 2005[1]

[1] Slides last updated on January 4, 2006

Outline

- Administrivia
- Machine learning: some basic definitions.
- Simple examples of regression.
- Real-world applications of regression.
- Simple examples of classification.
- Real-world applications of classification.

Administrivia

- Web page
  http://www.cs.ubc.ca/~murphyk/Teaching/Stat406_Spring06/index.html
- Please fill out the sign-up sheet.
- Labs Wed 4-5.
- The TA is Aline Tabet.
- My office hours are Fri 2-3pm LSK 308d.
- Aline's office hours are TBA (see web).

Grading

- There will be weekly homework assignments worth 20%.
  Out on Mondays, return on Mondays (in class).
- The homeworks will often involve programming; you may want to do this part during the lab.
- The midterm will be in late February and is worth 40%.
- The final will be in April and is worth 40%.

Pre-requisites

- Math: multivariate calculus, linear algebra, probability theory.
- Stats: stats 306 or CS 340 or equivalent.
- CS: some experience with programming (eg in R) is required.

Matlab

- There will be weekly programming assignments (as part of the lab).
- We will use matlab for programming.
- Matlab is very similar to R, but is somewhat faster and easier to learn. Matlab is widely used in the machine learning and Bayesian statistics community.
- Unfortunately matlab is not free (unlike R). You can buy a copy from the bookstore for $150, or you can use the copy installed in the lab machines.
- You will learn how to use matlab during the first few labs.

Textbook

- There is no official textbook. I will hand out various notes in class, including some chapters from the following unfinished/ unpublished books
  - *Probabilistic graphical models*, Michael Jordan, 2006
  - *Pattern recognition and machine learning*, Chris Bishop, 2006

  The following (already published) books are also recommended
  - *Elements of statistical learning*, Hastie, Friedman and Tibshirani, 2001. (Available from the bookstore)
  - *Pattern Classification*, Duda, Hart, Stork, 2001 (2nd edition).
  - *Statistical pattern recognition*, Andrew Webb, 2002.

Syllabus

- Since this is a new course, the syllabus is likely to change during the course of the semester.
- See the web page for details.
- You will get a good feeling for the class during today's lecture.

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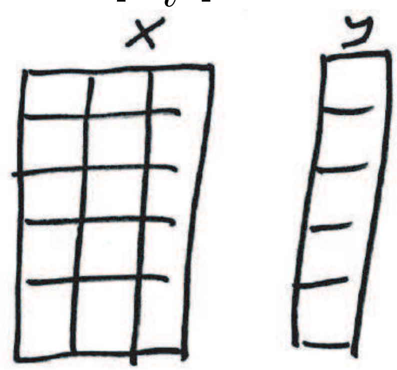
Learning to predict

- This class is about supervised approaches to machine learning.
- Given a training set of $n = N_D$ input-output pairs $D = (\vec{x}_i, \vec{y}_i)_{i=1}^{ND}$, we attempt to construct a function f which will accurately predict $f(\vec{x}_*)$ on future, test examples $\vec{x}_*$.
- Each input $\vec{x}_i$ is a vector of $p = N_X$ features or covariates. Each output $\vec{y}_i$ is a target variable. The training data is stored in an $N_D \times N_X$ design matrix $X = [\vec{x}_i^T]$. The training outputs are stored in a $N_D \times N_Y$ matrix $Y = [\vec{y}_i^T]$.



Classification vs regression

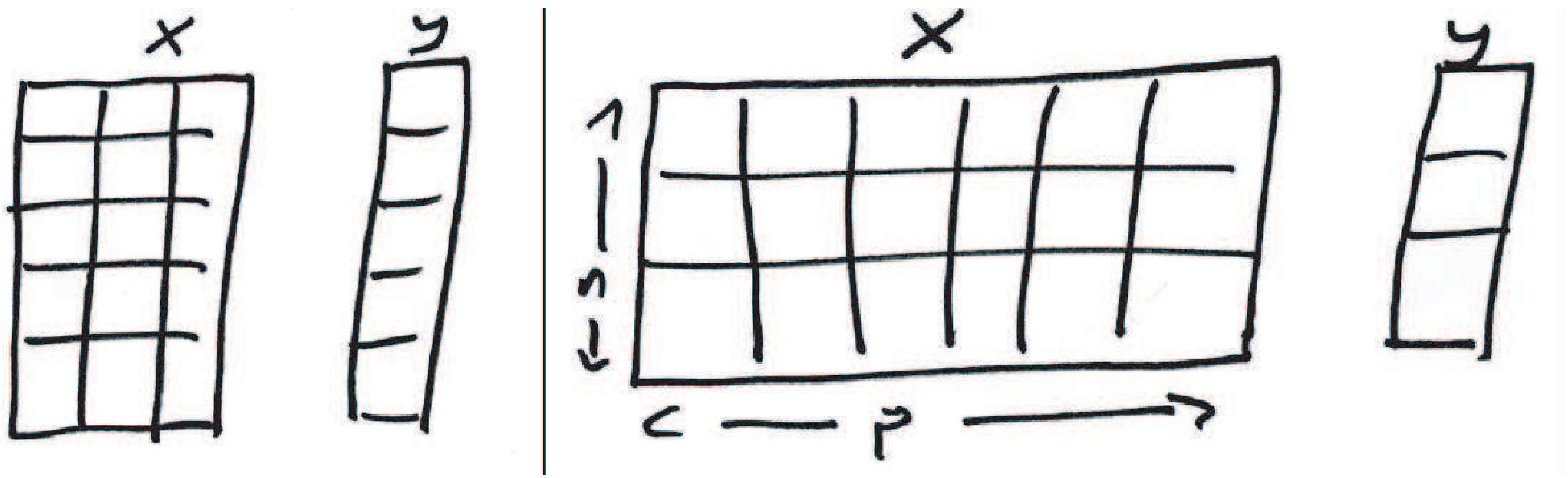
- If $\vec{y} \in \mathbb{R}^{N_Y}$ is a continuous-valued output, this is called **regression**. Often we will assume $N_Y = 1$, i.e., scalar output.
- If $y \in \{1, \ldots, N_Y\}$ is a discrete label, this is called **classification** or **pattern recognition**. The labels can be ordered (eg. low, medium, high) or unordered (e.g., male, female). N_Y is the number of classes. If $N_Y = 2$, this is called binary (dichotomous) classification.

Notation

- We will denote discrete ranges $\{1, \ldots, N\}$ by $1 : N$.
- We will often encode categorical variables as binary vectors. eg if $y \in \{1, \ldots, 3\}$, we will use $\vec{y} \in \{0,1\}^3$, where $y = 1$ maps to $\vec{y} = (1,0,0)$, $y = 2$ maps to $\vec{y} = (0,1,0)$, and $y = 3$ maps to $\vec{y} = (0,0,1)$.
- In general, $Y = j$ turns bit j of $\vec{Y}$ on, with the constraint $\sum_{j=1}^{N_Y} \vec{y} = 1$.

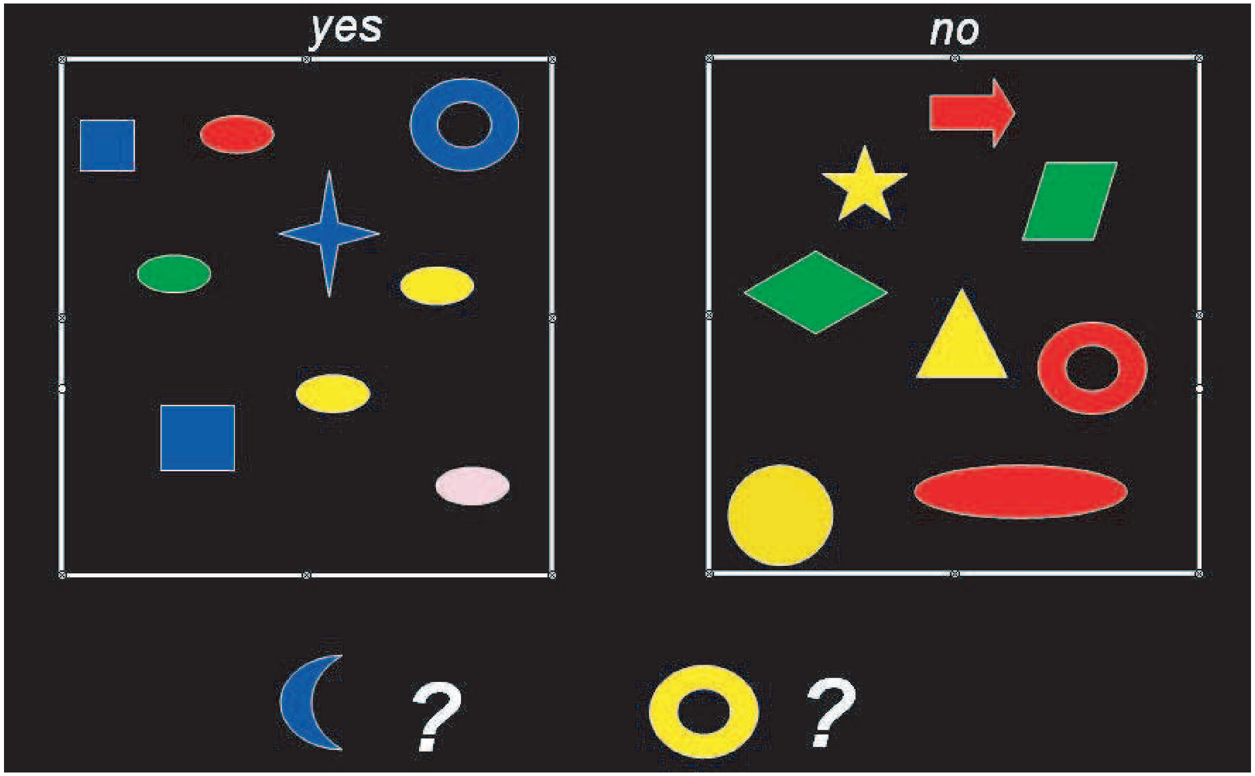
Short/fat vs tall/skinny data

- In traditional applications, the design matrix is tall and skinny ($n \gg p$), i.e., there are many more training examples than inputs.
- In more recent applications (eg. bio-informatics or text analysis), the design matrix is short and fat ($n \ll p$), so we will need to perform feature selection and/or dimensionality reduction.



Generalization performance

We care about performance on examples that are different from the training examples (so we can't just look up the answer).



No free lunch theorem

- The *no free lunch theorem* says (roughly) that there is no single method that is better at predicting across all possible data sets than any other method.
- Different learning algorithms implicitly make different assumptions about the nature of the data, and if they work well, it is because the assumptions are reasonable in a particular domain.

Supervised vs unsupervised learning

- In supervised learning, we are given $(\vec{x}_i, \vec{y}_i)$ pairs and try to learn how to predict $\vec{y}_*$ given $\vec{x}_*$.
- In unsupervised learning, we are just given $\vec{x}_i$ vectors.
- The goal in unsupervised learning is to learn a model that "explains" the data well. There are two main kinds:
  - Dimensionality reduction (eg PCA)
  - Clustering (eg K-means)

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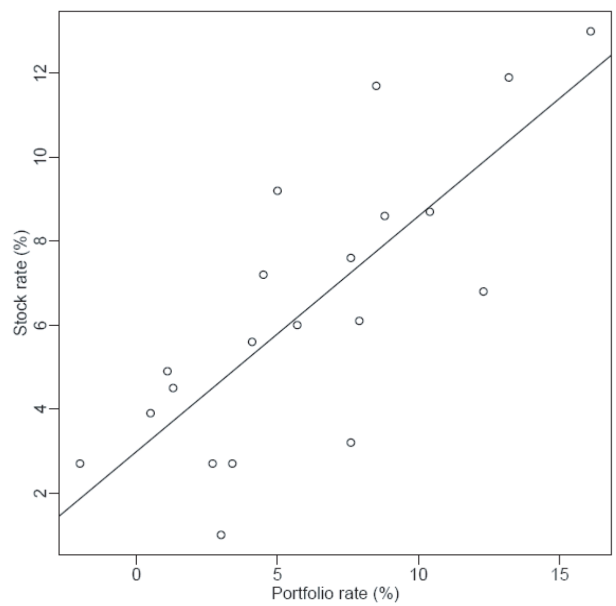
Linear regression

The output density is a 1D Gaussian (Normal) conditional on x:

$$p(y|\vec{x}) = \mathcal{N}(y; \vec{\beta}^T \vec{x}, \sigma) = \mathcal{N}(y; \beta_0 + \beta_1 x_1 + \cdots \beta_p x_p, \sigma)$$

$$\mathcal{N}(y|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp(-\frac{1}{2\sigma^2}(y-\mu)^T(y-\mu))$$

For example, $y = ax_1 + b$ is represented as $\vec{x} = (1, x_1)$ and $\vec{\beta} = (b, a)$.

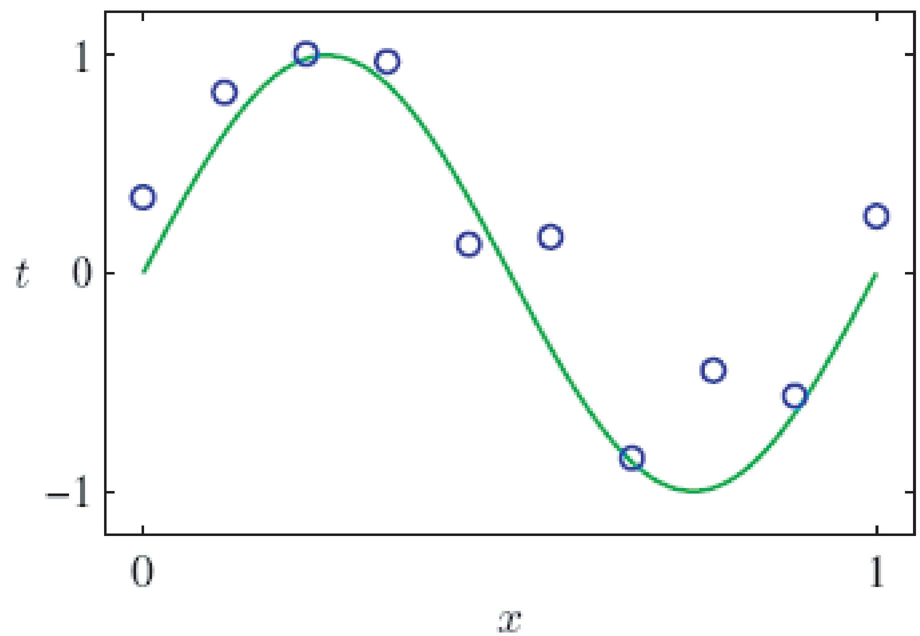


Polynomial regression

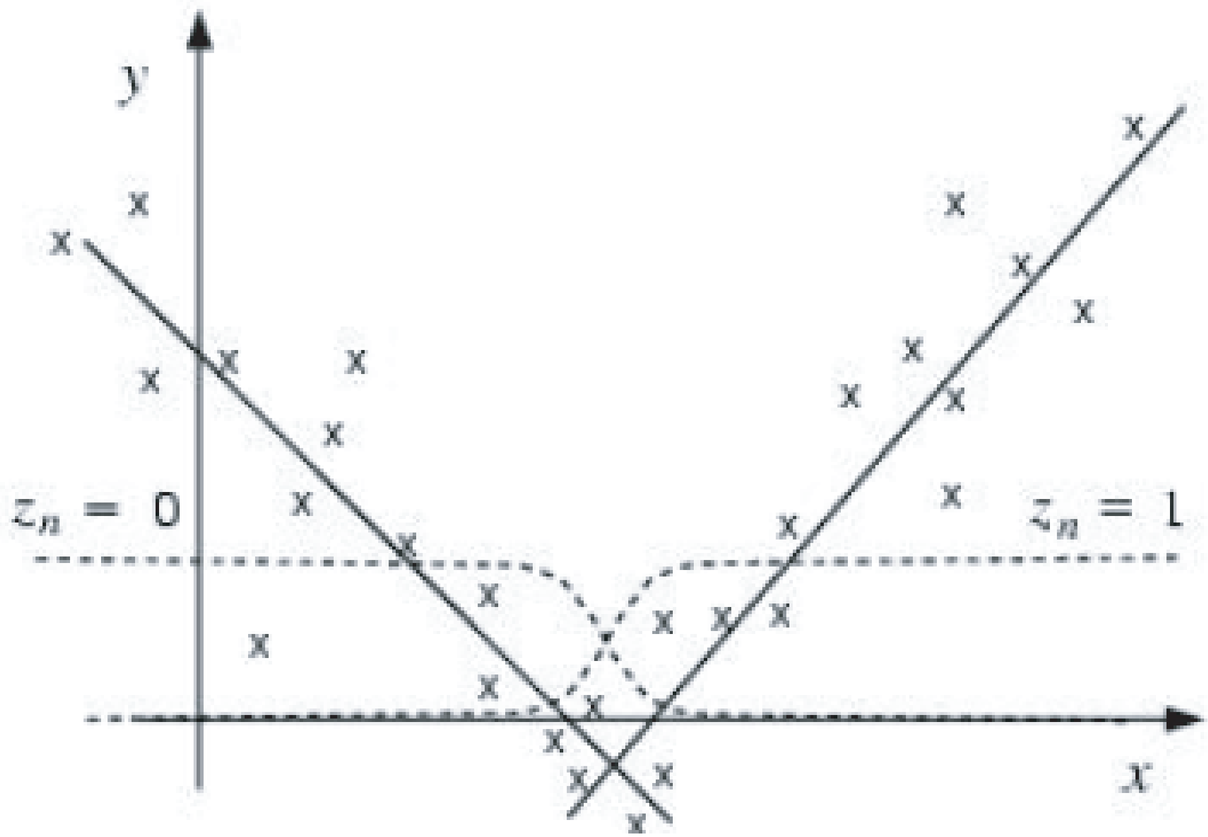
If we use linear regression with non-linear basis functions

$$p(y|x_1) = \mathcal{N}(y|\beta^T\,[1, x_1, x_1^2, \ldots, x_1^k], \sigma)$$

we can produce curves like the one below.
Note: In this class, we will often use $\vec{w}$ instead of $\vec{\beta}$ to denote the weight vector.



Piecewise linear regression



How many pieces? — Model selection problem.
Where to put them? — Segmentation problem.

2D LINEAR REGRESSION

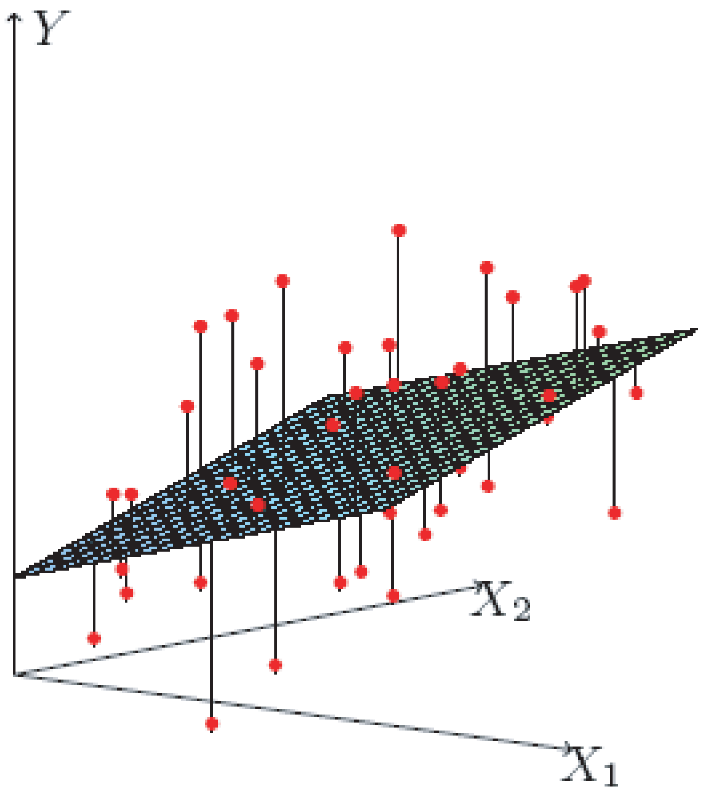


Figure 3.1: *Linear least squares fitting with* $X \in \mathbb{R}^2$. *We seek the linear function of* X *that minimizes the sum of squared residuals from* Y.

Piecewise linear 2D regression

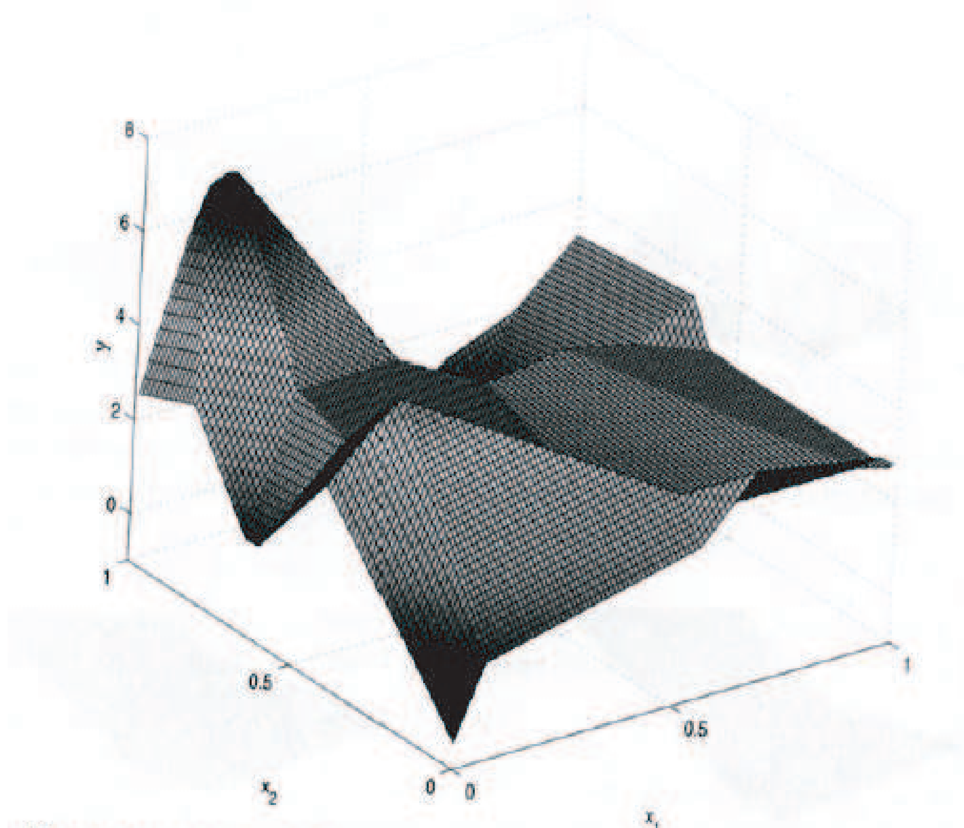


Figure 4.7 An example of a single realisation from a piecewise linear surface in two dimensions. (Reproduced by permission of the Royal Statistical Society.)

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Real-world applications of regression

- $\vec{x}$ = amount of various chemicals in my factory, y = amount of product produced.
- $\vec{x}$ = properties of a house (eg location, size), y = sales price.
- $\vec{x}$ = joint angles of my robot arm, $\vec{y}$ = location of arm in 3-space.
- $\vec{x}$ = stock prices today, $\vec{y}$ = stock prices tomorrow. (Time series data is not iid, and is beyond the scope of this course.)

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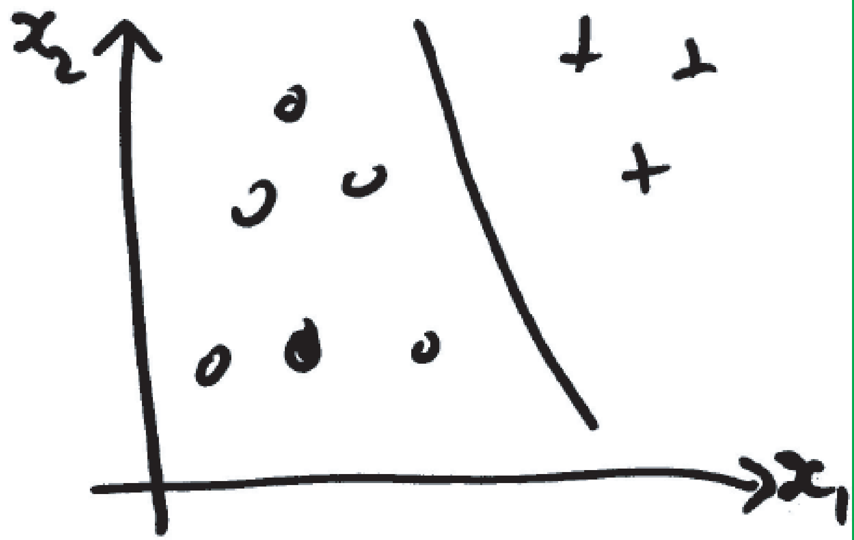
Linearly separable 2D data

2D inputs $\vec{x}_i \in \mathbb{R}^2$, binary outputs $y \in \{0, 1\}$.
The line is called a *decision boundary*.
Points to the right are classified as $y = 1$, points to the left as $y = 0$.



Logistic regression

- A simple approach to binary classification is logistic regression (briefly studied in 306).
- The output density is Bernoulli conditional on x:

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

where $y \in \{0, 1\}$ and

$$\pi(x) = \sigma(\vec{w}^T \, [1, x_1, x_2])$$

where

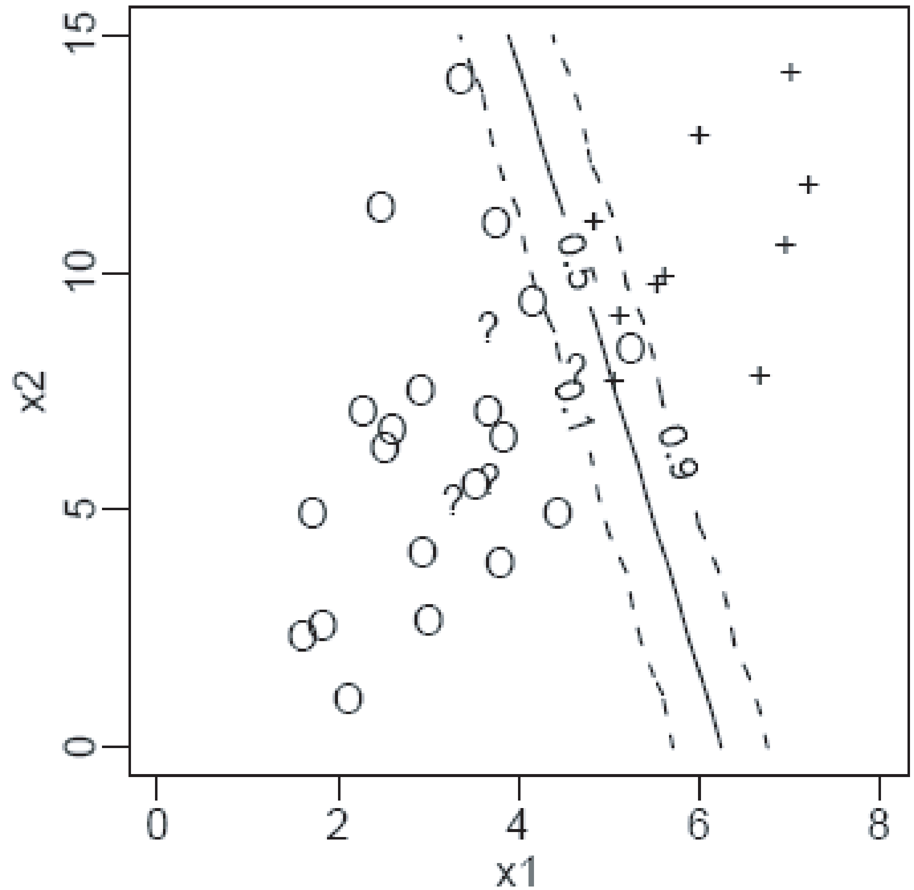
$$\sigma(u) = \frac{1}{1 + e^{-u}}$$

is the sigmoid (logistic) function that maps $\mathbb{R}$ to $[0, 1]$. Hence

$$P(Y = 1|\vec{x}) = \frac{1}{1 + e^{-w_0 + w_1 x_1 + w_2 x_2}}$$

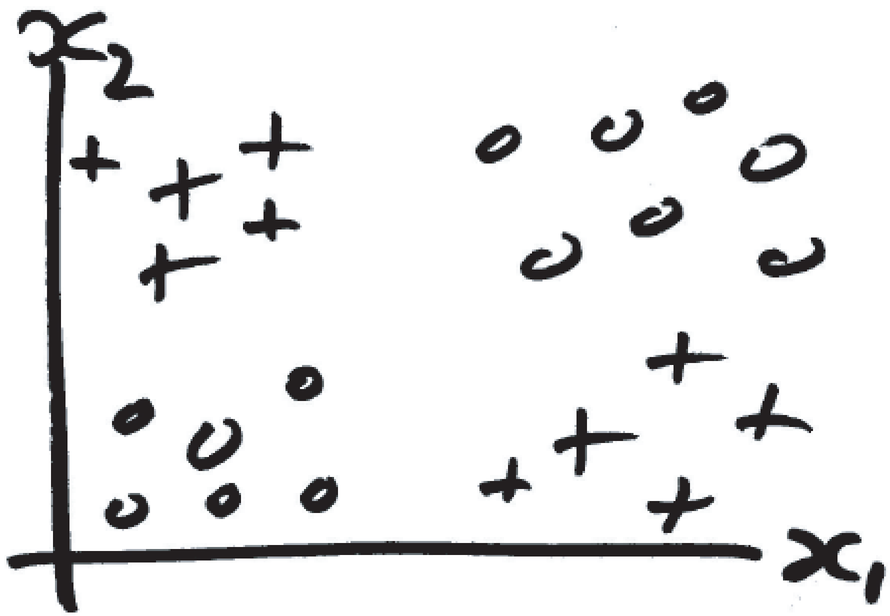
where w_0 is the bias (offset) term corresponding to the dummy column of 1s added to the design matrix.

2D Logistic regression



Non-linearly separable 2D data

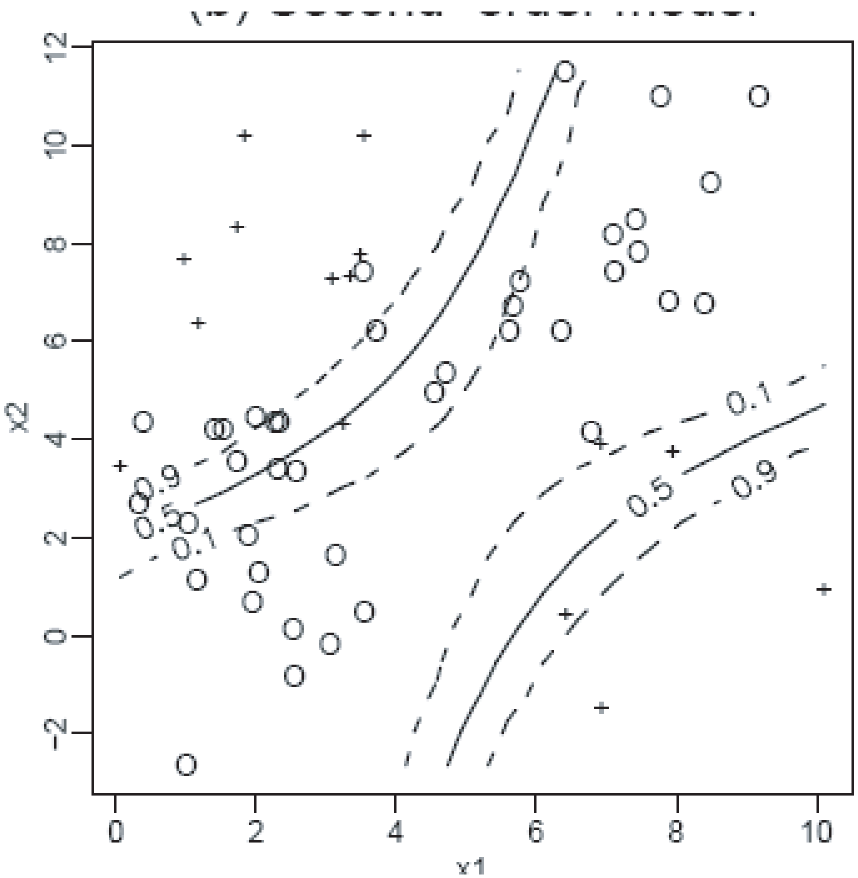
In 306, this is called "checkerboard" data.
In machine learning, this is called the "xor" problem.
The "true" function is $y = x_1 \oplus x_2$.
The decision boundary is non-linear.



Logistic regression with quadratic features

We can separate the classes using

$$P(Y=1|x_1,x_2) = \sigma(w^T\ [1, x_1, x_2, x_1^2, x_2^2, x_1, x_2])$$



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Handwritten digit recognition

Multi-class classification.

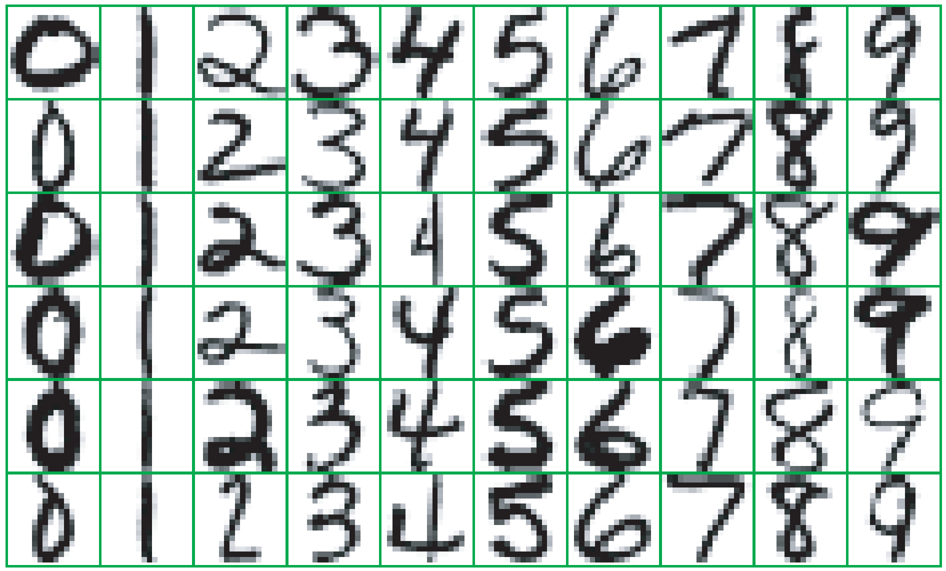
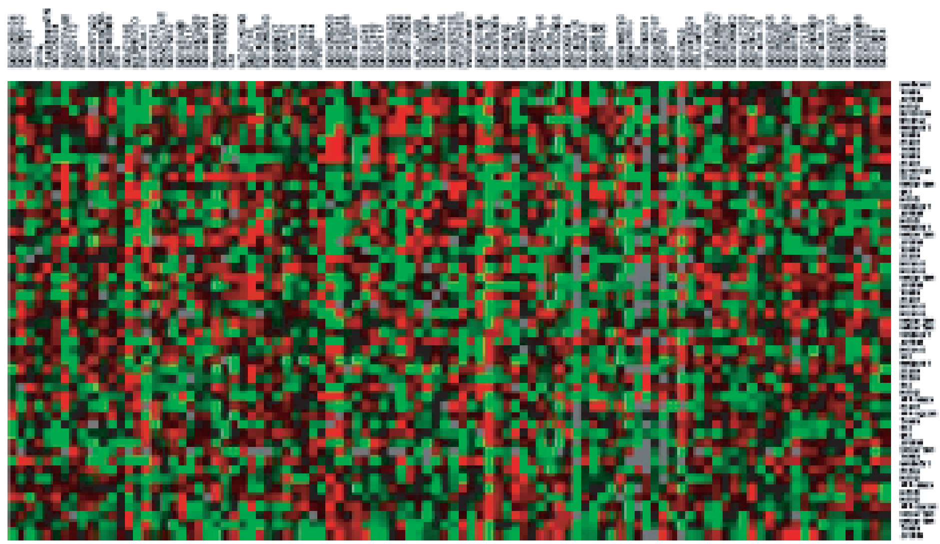


Figure 1.2: *Examples of handwritten digits from U.S. postal envelopes.*

Gene microarray expression data

Rows = examples, columns = features (genes).
Short, fat data ($p \gg N$).
Might need to perform feature selection.



Other examples of classification

- Email spam filtering (spam vs not spam)
- Detecting credit card fraud (fraudulent or legitimate)
- Face detection in images (face or background)
- Web page classification (sports vs politics vs entertainment etc)
- Steering an autonomous car across the US (turn left, right, or go straight)