Supervised Learning: Introduction

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Slides

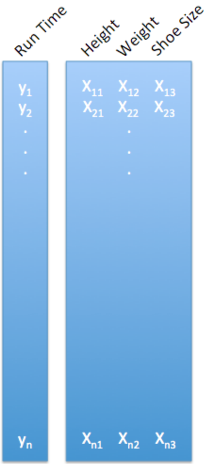
Slides and (some) codes are available at

`https://github.com/SISBID/Module4`

A Simple Example

- Suppose we have $n = 500$ kids for whom we have $p = 3$ measurements: height, weight, and shoe size.
- We wish to predict these kids' 1600-meter run times using these measurements.

A Simple Example



Notation:

- n is the number of observations.
- p the number of variables/features/predictors.
- y is a n-vector containing response/outcome for each of n observations.
- X is a $n \times p$ data matrix.

Linear Regression on a Simple Example

- You can perform linear regression to develop a model to predict run time using height, weight, and shoe size:

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \epsilon$$

where y is run time, X_1, X_2, X_3 are height, weight, and shoe size, and ϵ is a noise term.

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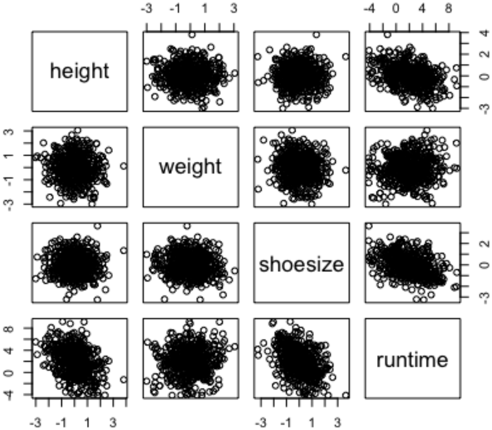
- You can look at the coefficients, p-values, and t-statistics for your linear regression model in order to interpret your results.
- You learned everything (or most of what) you need to analyze this data set in AP Statistics!

A Relationship Between the Variables?



Linear Model Output

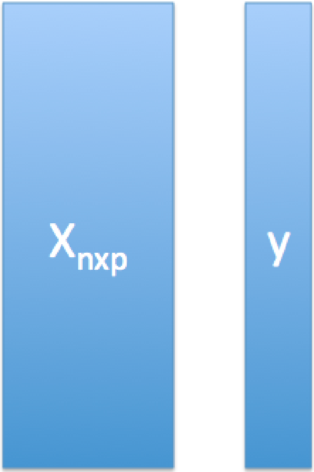
	Estimate	Std. Error	T-Stat	P-Value
Intercept	1.94179	0.09590	20.247	<2e-16 ***
height	-0.87704	0.09489	-9.243	<2e-16 ***
weight	0.07961	0.09105	0.874	0.382
shoesize	-1.00405	0.09530	-10.535	<2e-16 ***

$$\text{RunTime} \approx 1.94 - 0.88 \times \text{Height} + 0.08 \times \text{Weight} - 1.00 \times \text{ShoeSize}.$$

Low-Dimensional Versus High-Dimensional

- The data set that we just saw is low-dimensional: $n \gg p$.
- Lots of the data sets coming out of modern biological techniques are high-dimensional: $n \approx p$ or $n \ll p$.
- This poses statistical challenges! AP Statistics no longer applies.

Low Dimensional



High Dimensional

What Goes Wrong in High Dimensions?

- Suppose that we included many additional predictors in our model, such as
  - 50-yard dash time
  - Age
  - Zodiac symbol
  - Favorite color
  - Mother's birthday, in base 2

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- Overfitting: Model looks great on the data used to develop it, but will perform very poorly on future observations.

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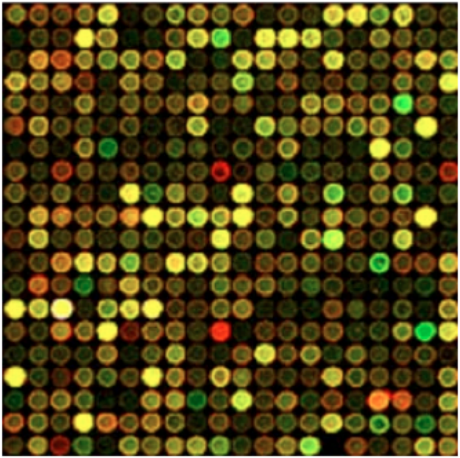
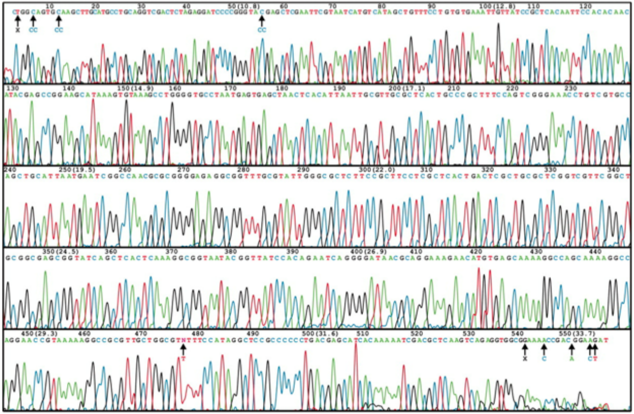
- Overfitting: Model looks great on the data used to develop it, but will perform very poorly on future observations.
- When $p \approx n$ or $p > n$, overfitting is guaranteed unless we are very careful.

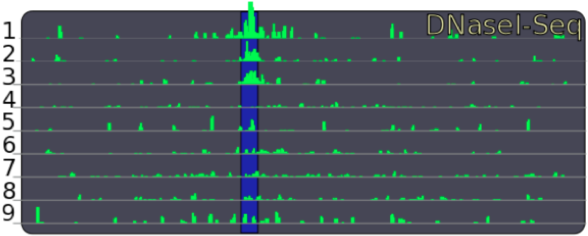
Gene Expression Data



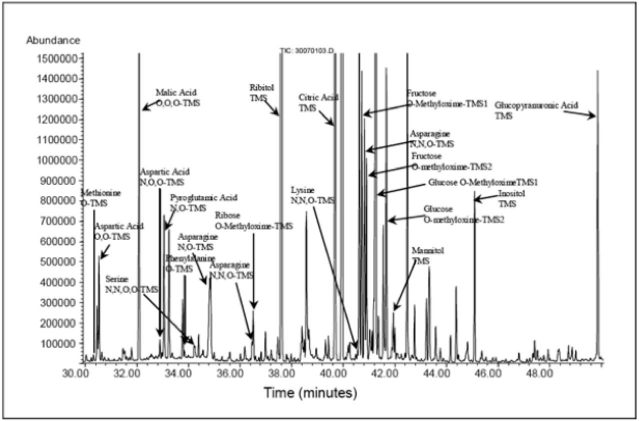
DNA Sequence Data



DNAse Hypersensitivity Data



Metabolomic Data



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- Cluster tissue samples on the basis of DNase hypersensitivity... using $n = 200$ cell types and $p = 1000000000$ variables.
- Identify genes whose expression is associated with survival time... using $n = 250$ cancer patients and $p = 20000$ variables.

Why Does Dimensionality Matter?

- Classical statistical techniques, such as linear regression, *cannot* be applied.
- Even very simple tasks, like identifying variables that are associated with a response, must be done with care.
- High risks of overfitting, false positives, and more.

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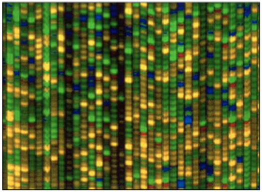
This course: Statistical machine learning tools for big – mostly high-dimensional – data.

Statistical Machine Learning



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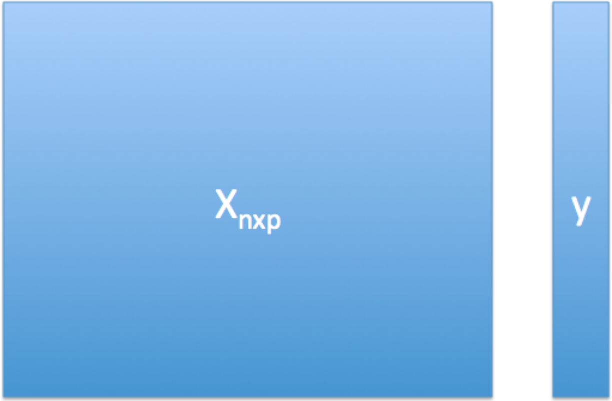
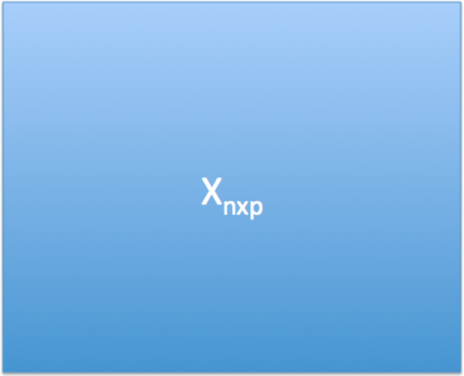
- Supervised Learning: Use a data set X to predict or detect association with a response y.
  - Regression
  - Classification
- Unsupervised Learning: Discover the signal in X, or detect associations within X.
  - Dimension Reduction
  - Clustering
  - Hypothesis Testing

Supervised Learning



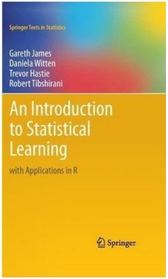
Unsupervised Learning



This Course

- We will cover the big ideas in supervised learning for big data.
- The best way to use these methods: learn R.

"Course Textbook" . . . with applications in R



- Available for (free!) download from www.statlearning.com.
- An accessible introduction to statistical machine learning, with an R lab at the end of each chapter!!
- We will go through some of these R labs in class.
- To learn more, go through them on your own!

Let's Try Out Some R!

Chapter 2 R lab
www.statlearning.com

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  - subtype of glioblastoma
- We will start with Regression.

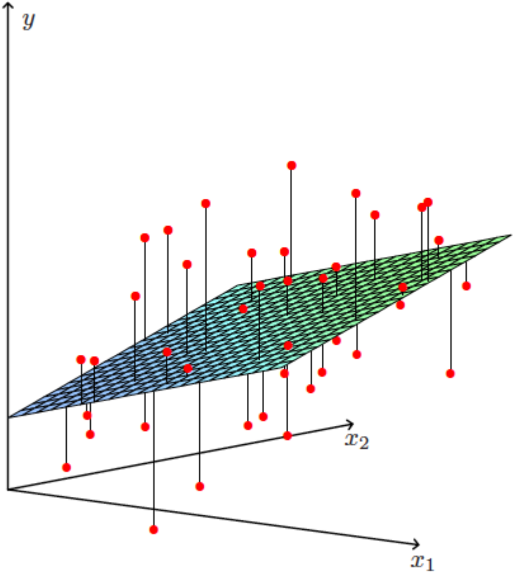
Linear Models

- We have n observations, for each of which we have p predictor measurements and a response measurement.
- Want to develop a model of the form

$$y_i = \beta_0 + \beta_1 X_{i1} + \cdots + \beta_p X_{ip} + \epsilon_i.$$

- Here ϵ_i is a noise term associated with the ith observation.
- Must estimate $\beta_0, \beta_1, \ldots, \beta_p$ — i.e. we must fit the model.

Linear Model With $p = 2$ Predictors



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- This is a linear model:

$$y_i = \beta_1 \sin(X_{i1}) + \beta_2 X_{i2} X_{i3} + \epsilon_i.$$

- This is not a linear model:

$$y_i = \beta_1^{X_{i1}} + \sin(\beta_2 X_{i2}) + \epsilon_i.$$

Linear Models in Matrix Form

- For simplicity, ignore the intercept β_0.
  - Assume $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} X_{ij} = 0$; in this case, $\beta_0 = 0$.
  - Alternatively, let the first column of X be a column of 1's.

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  - Alternatively, let the first column of X be a column of 1's.
- In matrix form, we can write the linear model as

$$\mathrm{y} = \mathrm{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

i.e.

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} X_{11} & X_{12} & \dots & X_{1p} \\ X_{21} & X_{22} & \dots & X_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ X_{n1} & X_{n2} & \dots & X_{np} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}.$$

Least Squares Regression

- There are a lot of ways we could fit the model $\mathrm{y} = \mathrm{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$.
- Most common approach in classical statistics is least squares:

$$\underset{\boldsymbol{\beta}}{\text{minimize}} \left\{ \|\mathrm{y} - \mathrm{X}\boldsymbol{\beta}\|^2 \right\}.$$

Here $\|\mathrm{a}\|^2 \equiv \sum_{i=1}^{n} a_i^2$.

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  Here $\|\mathrm{a}\|^2 \equiv \sum_{i=1}^n a_i^2$.
- We are looking for $\beta_1, \ldots, \beta_p$ such that

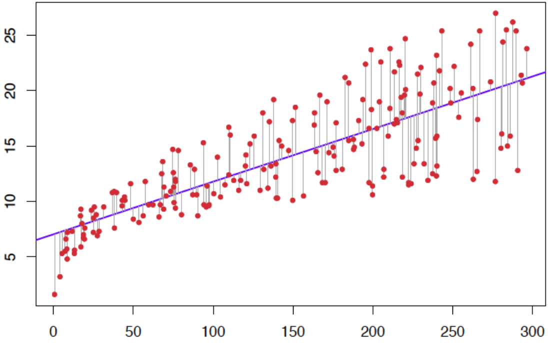
$$\sum_{i=1}^n (y_i - (\beta_1 X_{i1} + \cdots + \beta_p X_{ip}))^2$$

  is as small as possible.
- Equivalently, we're looking for coefficient estimates such that

$$\sum_{i=1}^n (y_i - \hat{y}_i)^2$$

  is as small as possible, where $\hat{y}_i$ is the ith predicted value.

Least Squares



- Horizontal axis: predictor
- Vertical axis: response
- Red dots: observations
- Purple line: least squares line

Purple line minimizes sum of squared lengths of the gray lines.

Let's Try Out Least Squares in R!

Chapter 3 R lab
www.statlearning.com