Introduction

Predictive Modeling & Statistical Learning

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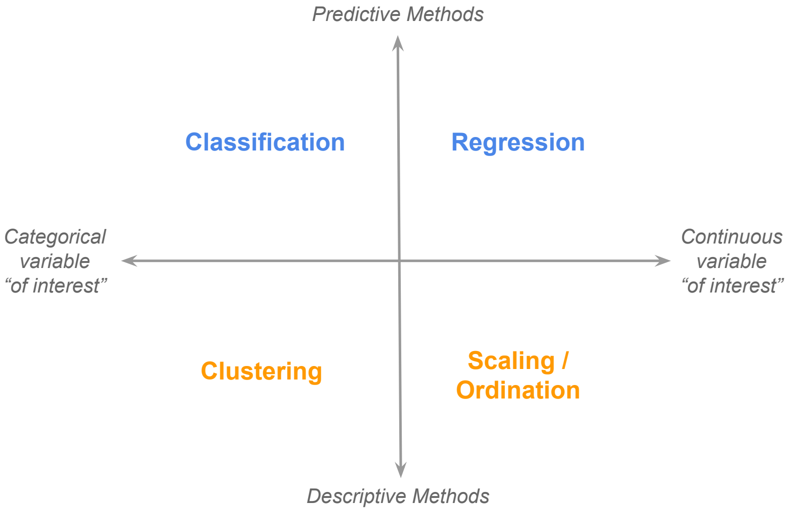
An introduction to Predictive Modeling and Statistical Learning

2 main branches:

Supervised -vs- Unsupervised

Statistics	Machine Learning
Predictive methods	Supervised learning
Descriptive methods	Unsupervised learning

Predictive and Descriptive Methods

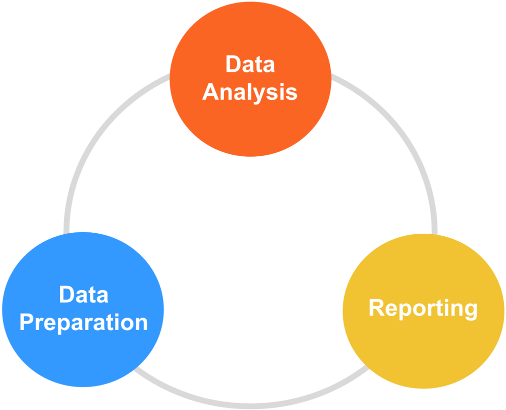


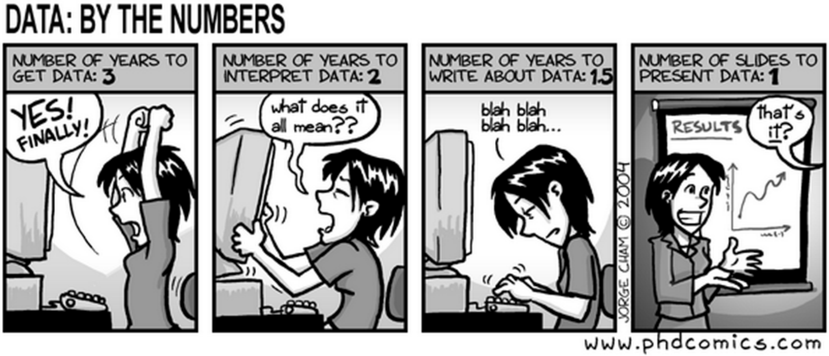
A word of caution

Sometimes there might not be a clear distinction between supervised and unsupervised learning. Often, a given method mixes both types of approaches.

Data Analysis Cycle (DAC)

Cycle of Data Anlaysis Projects





http://www.phdcomics.com/comics/archive.php/archive/tellafriend.php?comicid=462

Data Preparation

Core Data Analysis

Reporting

Communication

Major Data Analysis Tasks

- **Visualization**: to facilitate human discovery
- **Summarizing**: describing information
- **Deviation Detection**: finding changes
- **Profiling**: finding relevant characteristics of a group of individuals
- **Associations**: finding relationships, e.g. A & B & C occur frequently
- **Clustering**: finding groups in data

Major Data Analysis Tasks

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- **Clustering**: finding groups in data
- **Prediction**

Keep in mind

Data

Analysis

Report

Communication

Keep in mind

Data

Analysis

Report

Communication

This is where predictive modeling activities tend to take place

Keep in mind

Data

Analysis

Report

Communication

In practice these are where we spend most of our time

Modern Statistical Prediction?

- Statistical Prediction is not a new task
- Predictive applications date back to 18th century
- Regression framework originated at the beginning of 20th century (Francis Galton, Karl Pearson, Udny Yule)
- Classification framework originated around the 1930s (Ronald Fisher, P.C. Mahalanobis, B.L. Welch)

Modern Statistical Prediction

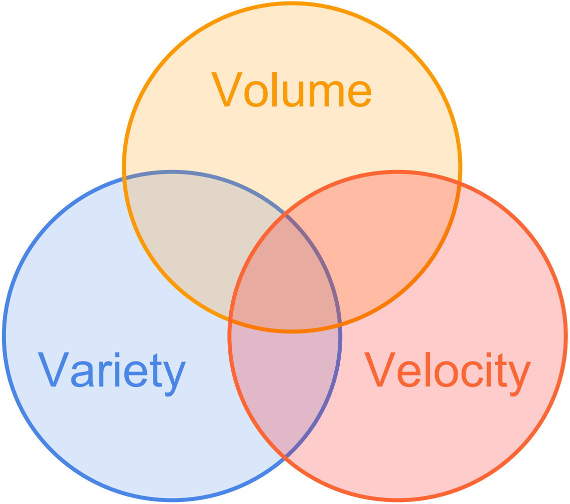
So where does the "modern" part come from?

- Data Sets
- Fields of Application
- Computing Tools
- Mathematical/Algorithmic Tweaks
- Predictive performance assessment
- Modeling Pipeline

So where does the “modern” part come from?

Data Sets

The three V's of Data

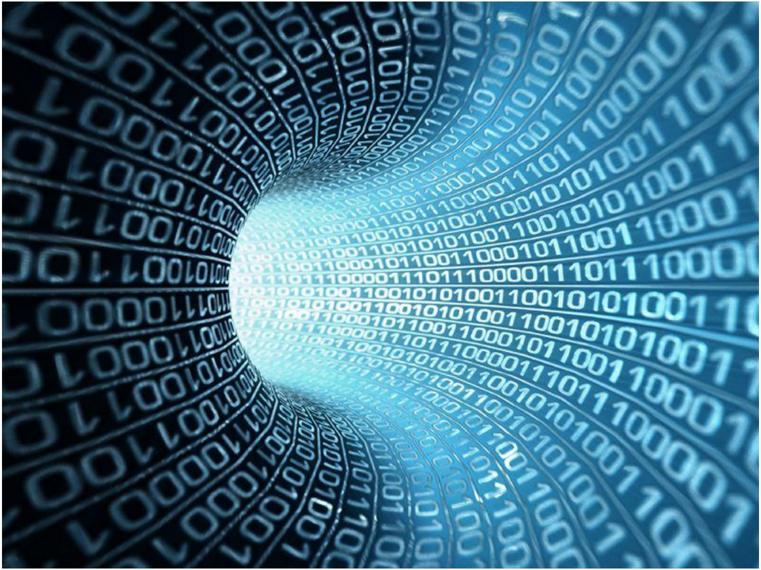


Modern Statistical Prediction?

The three V's

- **Volume**: larger data sets with reduced storage cost
- **Variety**: new types of data, more complex
- **Velocity**: increasing rate at which data is produced/recorded

Velocity

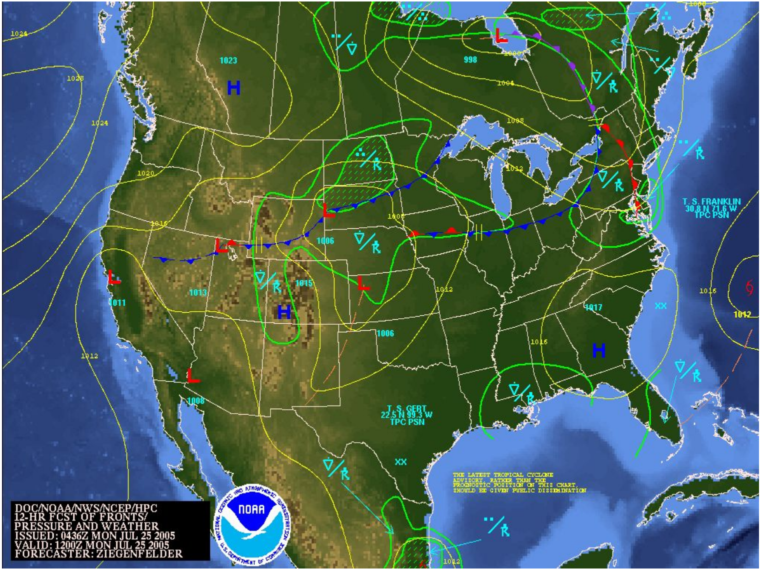


Volume

Variety

Variety

Variety


DOC/NOAA/NWS/NCEP/HPC
12-HR FCST OF FRONTS/
PRESSURE AND WEATHER
ISSUED: 0436Z MON JUL 25 2005
VALID: 1200Z MON JUL 25 2005
FORECASTER: ZIEGENFELDER
T. S. FRANKLIN
30.8 N 71.6 W
TPC PSN
T. S. GERT
22.5 N 99.3 W
TPC PSN
THE LATEST TROPICAL CYCLONE ADVISORY, RATHER THAN THE PROGNOSTIC POSITION ON THIS CHART, SHOULD BE GIVEN PUBLIC DISSEMINATION
NOAA

Variety


Linked in
skype
foursquare
YouTube
Insta
facebook
Blogger
my
twitter
flickr
tumblr.
yelp

So where does the “modern” part come from?

Fields of Application

Fields of Application Example

For instance, consider the history of PLS Regression (I'll talk about this with more detail when we study PLSR):

- Origins in mid-1960s with Herman Wold
- Wold deviced a series of algorithms based on Least Squares steps
- Applications in Psychometrics and Econometrics
- Wold's framework influenced by Joreskog's Structural Models with applications in Education, Sociology, Psychology
- Extension to multivariate regressions and systems of equations

Fields of Application Example (cont'd)

For instance, consider the history of PLS Regression (I'll talk about this with more detail when we study PLSR):

- Herman Wold's framework poorly unacknowledged (for various reasons)
- Applied to chemometrics in late 1970s
- Further adaptations by his son Svante Wold, and Harald Martens
- New regression approach by Partial Least Squares

So where does the “modern” part come from?

Mathematical/Algorithmic Tweaks

Mathematical/Algorithmic tweaks example

Multiple Linear Regression

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon$$

In matrix notation

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

Mathematical/Algorithmic tweaks example

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Predicted model

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}\mathbf{b}$$

Mathematical/Algorithmic tweaks example

OLS solution given by minimizing the residual sum of squares:

$$min \quad \sum_{i=1}^{n} \left(y_i - b_0 - \sum_{j=1}^{p} b_j x_j \right)^2$$

in vector-matrix notation:

$$min \quad \|\mathbf{y} - \mathbf{X}\mathbf{b}\|^2$$

Mathematical/Algorithmic tweaks example

Assuming that $\mathbf{X}$ is of full column-rank, the OLS solution for

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}\mathbf{b}$$

is given by:

$$\mathbf{b} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

Mathematical/Algorithmic tweaks example

Potential instability—due to multicollinearity—in the OLS solution affecting

$$(\mathbf{X}^\top \mathbf{X})^{-1}$$

Mathematical/Algorithmic tweaks example

One option: Find inverse of $(\mathbf{X}^\mathsf{T}\mathbf{X})$ by looking for an orthogonal basis:

$$(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1} = \mathbf{V}\boldsymbol{\Lambda}_*^\mathsf{T}\mathbf{V}^\mathsf{T}$$

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Another option: Modify $(\mathbf{X}^\mathsf{T}\mathbf{X})^{-\mathbf{1}}$ by adding a small constant k to the diagonal entries of $\mathbf{X}^\mathsf{T}\mathbf{X}$ before taking the inverse:

$$\mathbf{X}^\mathsf{T}\mathbf{X} + k\mathbf{I}$$

So where does the "modern" part come from?

Concept of "Predictive Modeling"

Goal Tradeoff

Understanding -vs- Prediction

Introduction

A statistical model typically aims to

Provide a certain comprehension of the data and the mechanism that generated them through a parsimonious representation of a random phenomenon.

Sometimes also, a statistical model seeks to

Predict new observations with “good” accuracy.

Understanding?

Understand could mean a model of a distribution for a random vector but it could also mean a regression model.

From a classic point of view, a model should be simple, and its parameters shuold be interpretable in terms of its domain of application (e.g. elasticity, odds-ratio, etc).

Predictive Modeling

The Process of developing a mathematical tool or model that generates an accurate prediction.

Kuhn and Johnson, 2013

Predictive Modeling

The art of building and using models that make predictions based on patterns extracted from historical data.

Kelleher et al, 2015

Paradox 1

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A "good" statistical model does not necessarily gives accurate predictions (at an individual level). E.g. risk factors in epidemiology.

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Paradox 2

We can predict without understanding

- no need for a theory of consumer to predict marketing target
- a model may be just simply an algorithm

Inference

Classic Inferential Statistics

Methodology for extracting information from data and expressing the amount of uncertainty in decisions we make.

- Assume distributions for the data
- Inferential aspects
- More theory-based
- More focused on testing hypotheses

So where does the “modern” part come from?

Assessing Predictive Performance

Model Performance

How do we define what a "good" model is?

- A model that fits the data well?
  (e.g. minimize resubstitution error)
- A model with optimal parameters?
  (e.g. most likely coefficients)
- A model that adequately predicts new (unseen) observations?
  (e.g. minimize generalization error)

Model Performance

- From the predictive modeling standpoint, a “good” model is one which gives accurate predictions.
- By *predictions* we mean predictions of new data.
- Therefore we focus on the generalization ability of the model to predict unobserved data
- This involves finding measure(s) of accuracy for predictions.

So where does the “modern” part come from?

Modeling Pipeline

Cycle of DAP and Predictive Modeling

- Data collection
- Data preparation (cleansing, formatting, transformations)
  - Feature selection
  - Feature extraction
- Model Building
  - Select modeling techniques
  - Select validation
  - Find optimal model
- Evaluation
- Deployment (decision making)

Predictive Modeling Process

Main Considerations

1. What data do you have?
2. What do you want to predict about the data?
3. What predictive methods/techniques should you use?
4. How accurate predictions look like?
5. What is the predictive performance?
6. Is there overfitting?

Terminology (Lebart, 1995)

Statistics	Machine Learning
Variables	Attributes (fields)
Individuals (objects, observations)	Instances (records, samples)
Predictors (independent)	Input
Response (dependent)	Output (target)
Model	Machine
Coefficients	Weights
Fit Criteria	Cost function
Estimation	Learning
Prediction	Supervised
Structure	Unsupervised

References

- **Modern Multivariate Statistical Techniques** by Izenman (2008). Springer.
- **Applied Predictive Modeling** by Kuhn and Johnson (2013).
- **Fundamentals for Machine Learning for Predictive Data Analytics** by Kelleher et al (2015).