### Lecture 1: Introduction



James D. Wilson
MSAN 628
Computational Statistics

### Plan for this Lecture



- A little about me
- Overview of Computational Statistics
  - Motivation and Applications
- Overview of this course

### A Little About Me



- Ph.D. Statistics and Operations Research (UNC Chapel Hill, '15)
  - Research focused on statistical analysis of networks
  - Explore, model, and analyze network data (e.g., social networks)
- M.S. Mathematical Sciences (Clemson University, '10)
- B.S. Mathematics and Chemistry (Campbell University '08)

### A Little About Me



#### Classes Lteach:

- BSDS 100 Intro to Data Science with R
- MATH 106 Business Statistics
- MATH 370 Probability with Applications
- MATH 373 Statistical Learning
- MSAN 601 Linear Regression Analysis
- MSAN 628 Computational Statistics
- MSAN 700 Social Network Analysis

### A Little About Me



- Born and raised in NC (near Raleigh)
- Live in Rockridge, Berkeley.
- A huge college basketball fan! (Go Heels!)
- Have loved college football since 2008 (Go Tigers!)
- Enjoy tasting beers (bourbon-barrel stouts are my favorite).
- I've always enjoyed teaching..

## Research that I work on: Network Analysis









## Network Anaylsis Research



- Significance-based community detection
- Generative models for fMRI correlation networks
- Network surveillance and changepoint analysis
- Effects of Networks on testing and inference
- Applications: Silicon Valley Wage Cartel, Urovirulence networks, Student social networks, etc.

### A Data Scientist's Toolkit



#### Harvard's data science toolkit:

- Wrangle the data: gather, clean, and sample data
- Manage the data: access big data quickly and reliably
- Explore the data: to make a hypothesis
- Make predictions: statistical methods
- Communicate the results: visualization, presentations, summaries

## What is Computational Statistics?



- "... the interface between statistics and computer science"
  - Wikipedia
- [2] "[A field devoted to] the design of algorithms for (1) implementing statistical methods on computers, including the ones unthinkable before the computer age and (2) coping with analytically intractable problems" - Carlo Lauro (IASC)

## What is Computational Statistics?



### Refers to computationally intensive statistical methods including

- resampling methods
- Markov chain Monte Carlo (MCMC) methods
- local regression
- kernel density estimation
- artificial neural networks
- generalized additive models

## A Major Component in Modern Data Science



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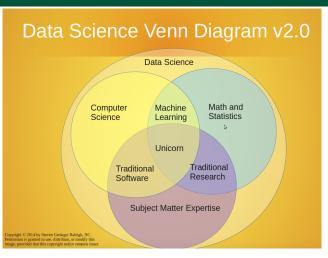


Figure: From www.datasciencecentral.com

Introduction

James D. Wilson (USF)

# Sample / Measurement Data



**Experiment:** Make *p* measurements on each of *n* samples.

**Result:** Data matrix / table X with n rows and p columns

- ith row of X is the vector of measurements on the ith sample
- jth column of X is the vector of values of the jth variable (measurement) across all samples

#### **Different Perspectives on data:**

- $n \times p$  matrix X
- n vectors of dimension p ⇔ samples
- p vectors of dimension n ⇔ variables

### **Notation**



Data matrix: 
$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}$$

**Rows of** *X*: *p* variable measurements for each observation.

$$x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^T$$

**Columns of** *X*: *n* observations of each variable.

$$\mathbf{x}_j = (x_{1j}, x_{2j}, \dots, x_{nj})^T$$

Can write *X* as: 
$$X = (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_p) = (x_1^T, x_2^T, ..., x_n^T)^T$$

## **Data Dimensionality**



**Old Paradigm:** More samples than variables (n >> p)

- Number of samples moderate (10s or 100s)
- Number of variables small (1s or 10s)

**High Dimensional Paradigm:** More variables than samples (p >> n)

- Number of samples moderate or large (100s or 1Ks)
- Number of variables very large (10Ks or 1Ms)

Big Data Paradigm: Many samples and/or many variables

Source of data: high-throughput measurement technologies for microarray analysis, e-commerce data, click-through rates, etc.

## Data Analytic Process



- Ask what kind of data? Supervised or unsupervised problem? What question are we trying to answer?
- Prepare / clean data: imputation, outlier removal, etc.
- Second Explore data → hypotheses about X and/or model f
- Apply models and algorithms to answer question
- Validation of approach

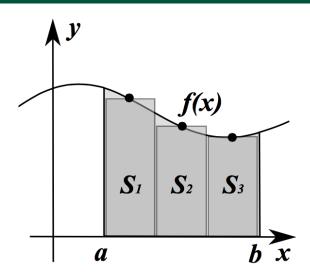
## Where Computational Statistics Comes In



- Imputation of missing data
- Approximating otherwise intractable functions
- Simulation
- Optimization / Estimation

## Example: Numerical Integration











#### **Variational Inference**

(in three easy steps...)

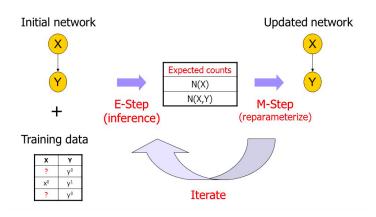
- Choose a family of variational distributions Q(H).
- 2. Use Kullback-Leibler divergence KL(Q||P) as a measure of 'distance' between P(H|D) and Q(H).
- 3. Find *Q* which minimizes divergence.

## Example: Imputation via the EM Algorithm





# Expectation Maximization (EM)



### **Great Resources**



- Flowingdata.com
  - Contemporary visualization and data manipulation techniques
- Kaggle.com
  - Kaggle competitions: win money for solving problems!
- Coursera.org
  - Free online courses in data science and machine learning
  - Recent notable course: "The Data Scientist's Toolbox"

# Primary books in this course





### Focus of this course...



### **Principles of Computational Statistics**

- Multivariate probability
- Bayesian computation (multivariate analysis)
- Algorithms: imputation, simulation, estimation, MCMC, EM, variational inference
- Theory: when to use an algorithm and why
- Software: R
- Data-driven

### ...so that we can do more than this...



