# Unsupervised Learning: Introduction

# About the Instructors

Genevera Allen:

- Columbia University - Department of Statistics.
- Member, Center for Theoretical Neuroscience; Zuckerman Institute for Mind, Brain, and Behavior; Irving Institute for Cancer Dynamics
- Research:
  - Statistical Machine Learning, Interpretable Machine Learning, Data Integration, Graphical Models, Modern Multivariate Analysis, Fairness, Neuroscience, Genomics.

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# About the Instructors

Yufeng Liu:

- University of North Carolina, Chapel Hill - Departments of Statistics and Operations Research, Genetics & Biostatistics.
- Research:
  - Statistical Machine Learning and Data Mining; High-dimensional Data Analysis; Nonparametric Statistics and Functional Estimation; Personalized Medicine; Bioinformatics.

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# Statistical Machine Learning

- "Learn" from current data to make predictions about the future.

  Examples?

- Intersection of: Computer Science, Statistics, Applied Math.

# Big Data

Big Data - BIG in Volume, Variety and/or Velocity (or Complexity!).

Common Big Data themes in Statistical Learning:

- Big $n$. Large number of observations.
  - Examples: Internet data, financial transactions, climate data, etc.
- Big $p$. Large number of features relative to observations. (High-dimensional data).
  - Examples: Medical data - genomics, neuroimaging, medical imaging, etc.

# Big Biomedical Data

Examples:

- High-throughput Genomics ("Omics").
  - RNA-sequencing, microarrays, methylation arrays, CGH-arrays, exome sequencing, mass spectrometry, NMR spectroscopy, etc.
- Neuroimaging / neural recordings.
  - MRI, Functional MRI (fMRI), EEG, MEG, DTI, ECoG, PET, etc.
- Electronic Health Records.
- Medical Imaging.
- Text Data - Pubmed abstracts.

# Data Matrix

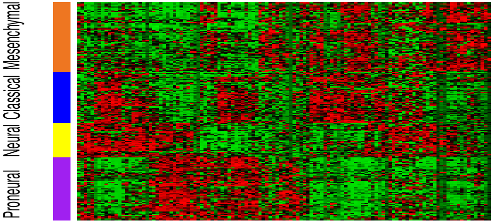
Data Matrix:

$$\boldsymbol{X}_{n\times p} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ \vdots & & \ddots & \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}$$

- Rows: $n$ observations / samples / subjects.
- Columns: $p$ features / variables.

# Data Matrix

Example: Omics Data




Gene Expression Data (Microarray)

- Rows (observations): Subjects ($n \approx 100 - 500$).
- Columns (features): Genes ($p \approx 500 - 20,000$).
- Measurement: Gene expression levels (loosely, how much a gene is turned off or on in a sample).

# Data Matrix

Example: Text Mining

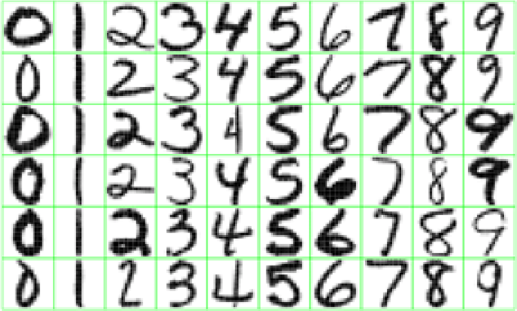
| | data | R | big | cluster | shiny | fast | plot |
|---|---|---|---|---|---|---|---|
| doc 1 | 57 | 1 | 43 | 2 | 0 | 22 | 4 |
| doc 2 | 17 | 29 | 2 | 3 | 35 | 6 | 44 |
| doc 3 | 47 | 33 | 0 | 0 | 24 | 3 | 19 |
| doc 4 | 23 | 0 | 0 | 31 | 0 | 7 | 2 |
| doc 5 | 40 | 5 | 28 | 9 | 0 | 21 | 6 |
| doc 6 | 8 | 10 | 7 | 46 | 12 | 17 | 9 |

(Bag-of-Words Format)

- Rows (observations): Documents ($n \approx 500 - 100,000$).
- Columns (features): Words ($n \approx 100 - 50,000$).
- Measurement: Count of how many times words appeared in documents.

# Data Matrix

Example: Image Data



(Handwritten Digits Data)

- Rows (observations): Digits ($n \approx 10,000$).
- Columns (features): Pixels ($p = 256$).
  - Each digit image is converted to a $16 \times 16$ grayscale image. The 256 total pixels are vectorized to form the features.
- Measurement: Normalized grayscale intensity of each pixel.

# Unsupervised vs. Supervised Learning

$$\boldsymbol{X}_{n \times p} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ \vdots & & \ddots & \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}$$

- Rows: $n$ observations / samples / subjects.
- Columns: $p$ features / variables.

Supervised Learning:

$$\mathbf{y} = (y_1, y_2, \dots y_n)^T$$

- $\mathbf{y}$ - $n$ labels / outcomes associated with each observation.

Unsupervised Learning: No outcomes / labels!

# Supervised Learning

## Main Goal

Prediction!

- Given: $(Y_n^{train}, \boldsymbol{X}_{n \times p}^{train})$ (Training Data).
- Training: Use training data to find $\hat{f}()$ that maps $\boldsymbol{X}$ to $Y$: $Y = f(\boldsymbol{X}) + \epsilon$.
- Prediction: Given new $\boldsymbol{X}_{m \times p}^{test}$, predict $Y_{m \times 1}^{test}$: $\hat{Y}^{test} = \hat{f}(\boldsymbol{X}^{test})$.

Examples?

Secondary Goals:

- Feature Selection - What features are associated with the outcome?
- Others?

# Unsupervised Learning

No labels! What is the goal?

**Main Goal**

Find some structure that characterizes the data.

(Or, find structure in training data that we expect to be present in future data.)

- Find patterns. (PCA, ICA, NMF, MDS)
- Dimension reduction. (PCA)
- Group observations / Group features / Group both. (Clustering)
- Find associations / relationships between features or observations. (Graphical or Network Models)
- Filter features. (Association testing)

# Unsupervised Learning

Challenges:

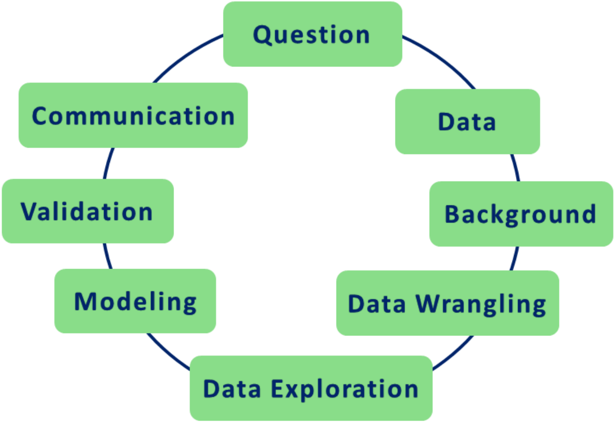
- Difficult to validate unsupervised learning results.
- No validation or test labels to measure prediction accuracy.
- What is meaningful structure in data?

Uses:

- Data pre-processing / compression / denoising.
- Exploratory data analysis.
  - Need to use multiple unsupervised learning techniques as each gives slightly different "insights" into data.
- Data visualization.
- Data-Driven Discovery.

# Unsupervised Learning

How does it fit into a data science pipeline?



# Unsupervised Learning

How is it used in Big Biomedical Data?

Case Study: BRCA gene expression data.

- Data Visualization.
  - Cluster heatmap, graphical models, MDS, PCA.
- Exploratory Analysis.
  - Clustering / dimension reduction to find cancer subtypes.
- Gene Selection.
  - Large-scale hypothesis testing to find genes associated with subtypes.
- Gene Interactions.
  - Graphical models.

# Breakout Discussion

- How will you use Unsupervised Learning?
- What type of big data do you work with?
- What do you hope to learn from this course?

# This Course

**Day 1:**

1. Lecture 1: 11:30-12:20pm - Intro
2. Lecture 2: 12:30-1:20pm - Dimension Reduction I
3. Lecture 3: 1:30-2:20pm - Dimension Reduction II/Lab Intro

**All times Pacific.*

# This Course

**Day 2:**

1. Lecture 1: 8-8:50am - Dimension Reduction III / Lab
2. Lecture 2: 9-9:50am - Dimension Reduction Lab
3. Lecture 3: 10-10:50am - Clustering I

Break

4. Lecture 4: 11:30-12:20pm - Clustering II
5. Lecture 5: 12:30-1:20pm - Clustering III / Lab
6. Lecture 6: 1:30-2:20pm - Clustering Lab

**All times Pacific.*

# This Course

**Day 3:**

1. Lecture 1: 8-8:50am - Testing
2. Lecture 2: 9-9:50am - Graphical Models I
3. Lecture 3: 10-10:50am - Graphical Models II

Break

4. Lecture 4: 11:30-12:20pm - Validation + Final Lab
5. Lecture 5: 12:30-1:20pm - Final Lab
6. Lecture 6: 1:30-2:20pm - Final Lab Results + Best Practices

**All times Pacific.*