## Lecture 1: Introduction

#### Nayel Bettache

Department of Statistical Science, Cornell University

"Artificial intelligence (or machine learning) is actually statistics, but it uses a very gorgeous rhetoric. It is actually statistics. A lot of formulas are very old. But all artificial intelligence uses statistics to solve problems."

-Thomas J. Sargent, Nobel Prize winner in Economics, 2018

"Artificial intelligence (or machine learning) is actually statistics, but it uses a very gorgeous rhetoric. It is actually statistics. A lot of formulas are very old. But all artificial intelligence uses statistics to solve problems."

-Thomas J. Sargent, Nobel Prize winner in Economics, 2018

"When you are fundraising, it is AI. When you are hiring, it is ML. When you are implementing, it is logistic regression."

-everyone on Twitter ever

## Machine Learning (ML) vs Stat



Comic copyright Thomas Wiecki, Ph.D., ODSC Europe 2018

• Statistical learning involves tools for understanding data.

- Statistical learning involves tools for understanding data.
- Methods are categorized as:

- Statistical learning involves tools for understanding data.
- Methods are categorized as:
  - **Supervised learning**: Builds models to predict or estimate an output based on input data.

- Statistical learning involves tools for understanding data.
- Methods are categorized as:
  - **Supervised learning**: Builds models to predict or estimate an output based on input data.
  - **Unsupervised learning**: Discovers relationships and structures in data without an output variable.

- Statistical learning involves tools for understanding data.
- Methods are categorized as:
  - **Supervised learning**: Builds models to predict or estimate an output based on input data.
  - **Unsupervised learning**: Discovers relationships and structures in data without an output variable.
- Applications span across diverse fields such as business, medicine, astrophysics, and public policy.

• Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Focus on relationships between:



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Focus on relationships between:
  - Age and wage: Wages increase with age, then decline after age 60.



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Focus on relationships between:
  - Age and wage: Wages increase with age, then decline after age 60.
  - Year and wage: Slight wage increase between 2003 and 2009.



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Focus on relationships between:
  - Age and wage: Wages increase with age, then decline after age 60.
  - Year and wage: Slight wage increase between 2003 and 2009.
  - Education and wage: Higher education correlates with higher wages.



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Age alone isn't a precise predictor due to high variability.



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Age alone isn't a precise predictor due to high variability.
- Best wage predictions combine age, education, and year.



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Age alone isn't a precise predictor due to high variability.
- Best wage predictions combine age, education, and year.
- Linear regression can be used to predict wage from this data set (next chapter).



- Wage data set: Analyzes factors influencing wages for men in the Atlantic region of the U.S.
- Age alone isn't a precise predictor due to high variability.
- Best wage predictions combine age, education, and year.
- Linear regression can be used to predict wage from this data set (next chapter).
- Ideally, we should predict wage in a way that accounts for the non-linear relationship between wage and age.



• Smarket data set: Analyzes daily movements of the S&P 500 index over a 5-year period.



- Smarket data set: Analyzes daily movements of the S&P 500 index over a 5-year period.
- Goal: Predict index mvmt based on the previous days' percentage changes.



- Smarket data set: Analyzes daily movements of the S&P 500 index over a 5-year period.
- Goal: Predict index mvmt based on the previous days' percentage changes.
- Left-hand panel: Boxplots for the previous day's percentage change.



- Smarket data set: Analyzes daily movements of the S&P 500 index over a 5-year period.
- Goal: Predict index mvmt based on the previous days' percentage changes.
- Left-hand panel: Boxplots for the previous day's percentage change.
- Little difference between days the market increased vs. decreased, suggesting no simple predictive strategy.



• Predicts a continuous or quantitative output.

- Predicts a continuous or quantitative output.
- Example: Wage data set where the goal is to predict wages based on factors like age and education.

- Predicts a continuous or quantitative output.
- Example: Wage data set where the goal is to predict wages based on factors like age and education.
- Classification Problem:

- Predicts a continuous or quantitative output.
- Example: Wage data set where the goal is to predict wages based on factors like age and education.

#### • Classification Problem:

• Predicts a categorical or qualitative outcome.

- Predicts a continuous or quantitative output.
- Example: Wage data set where the goal is to predict wages based on factors like age and education.

#### • Classification Problem:

- Predicts a categorical or qualitative outcome.
- Example: Smarket data set, predicting whether the S&P 500 index will increase (Up) or decrease (Down) on a given day.

• NCI60 data set: Contains 6,830 gene expression measurements for 64 cancer cell lines.



- NCI60 data set: Contains 6,830 gene expression measurements for 64 cancer cell lines.
- Goal: Determine clusters among cell lines based on gene expression data.



- NCI60 data set: Contains 6,830 gene expression measurements for 64 cancer cell lines.
- Goal: Determine clusters among cell lines based on gene expression data.
- We apply Principal Component Analysis (PCA)



- NCI60 data set: Contains 6,830 gene expression measurements for 64 cancer cell lines.
- Goal: Determine clusters among cell lines based on gene expression data.
- We apply Principal Component Analysis (PCA)
- Reduces 6,830 measurements to two principal components (Z1 and Z2).



- NCI60 data set: Contains 6,830 gene expression measurements for 64 cancer cell lines.
- Goal: Determine clusters among cell lines based on gene expression data.
- We apply Principal Component Analysis (PCA)
- Reduces 6,830 measurements to two principal components (Z1 and Z2).
- Allows visualization of potential clusters in a 2D space.



- NCI60 data set: Contains 6,830 gene expression measurements for 64 cancer cell lines.
- Goal: Determine clusters among cell lines based on gene expression data.
- We apply Principal Component Analysis (PCA)
- Reduces 6,830 measurements to two principal components (Z1 and Z2).
- Allows visualization of potential clusters in a 2D space.
- Some information loss is expected, but clustering is now visually assessable.



• Left: Rep. of the NCI60 gene expression data set in a 2D space.



- Left: Rep. of the NCI60 gene expression data set in a 2D space.
- Each point corresponds to one of the 64 cell lines


#### Gene Expression Data

- Left: Rep. of the NCI60 gene expression data set in a 2D space.
- Each point corresponds to one of the 64 cell lines
- Suggests at least four clusters among the cell lines.



### Gene Expression Data

- Left: Rep. of the NCI60 gene expression data set in a 2D space.
- Each point corresponds to one of the 64 cell lines
- Suggests at least four clusters among the cell lines.
- Right: Same but displays 14 cancer types using distinct colored symbols.



### Gene Expression Data

- Left: Rep. of the NCI60 gene expression data set in a 2D space.
- Each point corresponds to one of the 64 cell lines
- Suggests at least four clusters among the cell lines.
- Right: Same but displays 14 cancer types using distinct colored symbols.
- Shows that cell lines with the same cancer type are often near each other.



• Wage and Smarket data sets contain both input and output variables.

- Wage and Smarket data sets contain both input and output variables.
- Another important class of problems involves situations in which we only observe input variables, with no corresponding output.

- Wage and Smarket data sets contain both input and output variables.
- Another important class of problems involves situations in which we only observe input variables, with no corresponding output.
- Example: Marketing setting where customers are grouped based on demographic data.

- Wage and Smarket data sets contain both input and output variables.
- Another important class of problems involves situations in which we only observe input variables, with no corresponding output.
- Example: Marketing setting where customers are grouped based on demographic data.
- Goal: Identify groups or clusters of similar individuals based on observed characteristics.

### Supervised learning problem

• The dataset contains *n* observations.

## Supervised learning problem

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.

## Supervised learning problem

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem, *y<sub>i</sub>* takes values in a finite, unordered set (e.g. up/down).

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem,  $y_i$  takes values in a finite, unordered set (e.g. up/down).
- For each observation, there is a vector of p predictor measurements, usually called inputs or regressors or covariates or features or independent variables and denoted  $x_i$  where i = 1, ..., n (e.g. age, year, education level).

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem,  $y_i$  takes values in a finite, unordered set (e.g. up/down).
- For each observation, there is a vector of p predictor measurements, usually called inputs or regressors or covariates or features or independent variables and denoted  $x_i$  where i = 1, ..., n (e.g. age, year, education level).
- The observed training data  $(x_1, y_1), \ldots, (x_n, y_n)$  are usually called samples or instances.

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem,  $y_i$  takes values in a finite, unordered set (e.g. up/down).
- For each observation, there is a vector of p predictor measurements, usually called inputs or regressors or covariates or features or independent variables and denoted  $x_i$  where i = 1, ..., n (e.g. age, year, education level).
- The observed training data  $(x_1, y_1), \ldots, (x_n, y_n)$  are usually called samples or instances.
- Based on the observed data we would like to perform:

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem,  $y_i$  takes values in a finite, unordered set (e.g. up/down).
- For each observation, there is a vector of p predictor measurements, usually called inputs or regressors or covariates or features or independent variables and denoted  $x_i$  where i = 1, ..., n (e.g. age, year, education level).
- The observed training data  $(x_1, y_1), \ldots, (x_n, y_n)$  are usually called samples or instances.
- Based on the observed data we would like to perform:
  - Prediction: accurately predict future outcome.

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem,  $y_i$  takes values in a finite, unordered set (e.g. up/down).
- For each observation, there is a vector of p predictor measurements, usually called inputs or regressors or covariates or features or independent variables and denoted  $x_i$  where i = 1, ..., n (e.g. age, year, education level).
- The observed training data  $(x_1, y_1), \ldots, (x_n, y_n)$  are usually called samples or instances.
- Based on the observed data we would like to perform:
  - Prediction: accurately predict future outcome.
  - Estimation: understand how inputs affect the outcome.

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem,  $y_i$  takes values in a finite, unordered set (e.g. up/down).
- For each observation, there is a vector of p predictor measurements, usually called inputs or regressors or covariates or features or independent variables and denoted  $x_i$  where i = 1, ..., n (e.g. age, year, education level).
- The observed training data  $(x_1, y_1), \ldots, (x_n, y_n)$  are usually called samples or instances.
- Based on the observed data we would like to perform:
  - Prediction: accurately predict future outcome.
  - Estimation: understand how inputs affect the outcome.
  - Model selection: find the best model for the outcome or which inputs affect the outcome.

- The dataset contains *n* observations.
- For each observation, there is an outcome measurement, usually called dependent variable or response or target and noted  $y_i$  where i = 1, ..., n.
  - In the regression problem,  $y_i$  is quantitative (e.g wage).
  - In the classification problem,  $y_i$  takes values in a finite, unordered set (e.g. up/down).
- For each observation, there is a vector of p predictor measurements, usually called inputs or regressors or covariates or features or independent variables and denoted  $x_i$  where i = 1, ..., n (e.g. age, year, education level).
- The observed training data  $(x_1, y_1), \ldots, (x_n, y_n)$  are usually called samples or instances.
- Based on the observed data we would like to perform:
  - Prediction: accurately predict future outcome.
  - Estimation: understand how inputs affect the outcome.
  - Model selection: find the best model for the outcome or which inputs affect the outcome.
  - Inference: assess the quality of our predictions.

• The dataset contains *n* observations.

- The dataset contains *n* observations.
- For each observation, there is no outcome measurement

- The dataset contains *n* observations.
- For each observation, there is no outcome measurement
- For each observation, there is a vector of *p* predictor measurements denoted *x<sub>i</sub>* where *i* = 1,..., *n* (e.g.gene expression measurements).

- The dataset contains *n* observations.
- For each observation, there is no outcome measurement
- For each observation, there is a vector of *p* predictor measurements denoted *x<sub>i</sub>* where *i* = 1,..., *n* (e.g.gene expression measurements).
- The objective is here more fuzzy. We can be interested on

- The dataset contains *n* observations.
- For each observation, there is no outcome measurement
- For each observation, there is a vector of *p* predictor measurements denoted *x<sub>i</sub>* where *i* = 1,..., *n* (e.g.gene expression measurements).
- The objective is here more fuzzy. We can be interested on
  - Finding groups of samples that behave similarly.

- The dataset contains *n* observations.
- For each observation, there is no outcome measurement
- For each observation, there is a vector of *p* predictor measurements denoted *x<sub>i</sub>* where *i* = 1,..., *n* (e.g.gene expression measurements).
- The objective is here more fuzzy. We can be interested on
  - Finding groups of samples that behave similarly.
  - Find linear combinations of features with the most variation.

- The dataset contains *n* observations.
- For each observation, there is no outcome measurement
- For each observation, there is a vector of *p* predictor measurements denoted *x<sub>i</sub>* where *i* = 1,..., *n* (e.g.gene expression measurements).
- The objective is here more fuzzy. We can be interested on
  - Finding groups of samples that behave similarly.
  - Find linear combinations of features with the most variation.
  - Other

- The dataset contains *n* observations.
- For each observation, there is no outcome measurement
- For each observation, there is a vector of *p* predictor measurements denoted *x<sub>i</sub>* where *i* = 1,..., *n* (e.g.gene expression measurements).
- The objective is here more fuzzy. We can be interested on
  - Finding groups of samples that behave similarly.
  - Find linear combinations of features with the most variation.
  - Other
- The model assessment problem is difficult as it is hard to know how well you are doing.

• It is important to understand the ideas behind the various techniques, in order to know how and when to use them.

- It is important to understand the ideas behind the various techniques, in order to know how and when to use them.
- One has to understand the simpler methods first, in order to grasp the more sophisticated ones.

- It is important to understand the ideas behind the various techniques, in order to know how and when to use them.
- One has to understand the simpler methods first, in order to grasp the more sophisticated ones.
- It is important to accurately assess the performance of a method, to know how well or how badly it is working. Simpler methods sometimes perform as well as fancier ones.

- It is important to understand the ideas behind the various techniques, in order to know how and when to use them.
- One has to understand the simpler methods first, in order to grasp the more sophisticated ones.
- It is important to accurately assess the performance of a method, to know how well or how badly it is working. Simpler methods sometimes perform as well as fancier ones.
- This is an exciting research area, having important applications in science, industry and finance.

- It is important to understand the ideas behind the various techniques, in order to know how and when to use them.
- One has to understand the simpler methods first, in order to grasp the more sophisticated ones.
- It is important to accurately assess the performance of a method, to know how well or how badly it is working. Simpler methods sometimes perform as well as fancier ones.
- This is an exciting research area, having important applications in science, industry and finance.
- Statistical learning is a fundamental ingredient in the training of a modern data scientist.

• Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.
- 1940s: various authors put forth an alternative approach, logistic regression.
- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.
- 1940s: various authors put forth an alternative approach, logistic regression.
- Early 1970s: the term generalized linear model was developed to describe an entire class of statistical learning methods that include both linear and logistic regression as special cases.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.
- 1940s: various authors put forth an alternative approach, logistic regression.
- Early 1970s: the term generalized linear model was developed to describe an entire class of statistical learning methods that include both linear and logistic regression as special cases.
- Late 1970s: more techniques for learning from data were available.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.
- 1940s: various authors put forth an alternative approach, logistic regression.
- Early 1970s: the term generalized linear model was developed to describe an entire class of statistical learning methods that include both linear and logistic regression as special cases.
- Late 1970s: more techniques for learning from data were available.
- However, they were almost exclusively linear methods be- cause fitting non-linear relationships was computationally difficult at the time.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.
- 1940s: various authors put forth an alternative approach, logistic regression.
- Early 1970s: the term generalized linear model was developed to describe an entire class of statistical learning methods that include both linear and logistic regression as special cases.
- Late 1970s: more techniques for learning from data were available.
- However, they were almost exclusively linear methods be- cause fitting non-linear relationships was computationally difficult at the time.
- Mid 1980s, classification and regression trees were developed, followed shortly by generalized additive models.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.
- 1940s: various authors put forth an alternative approach, logistic regression.
- Early 1970s: the term generalized linear model was developed to describe an entire class of statistical learning methods that include both linear and logistic regression as special cases.
- Late 1970s: more techniques for learning from data were available.
- However, they were almost exclusively linear methods be- cause fitting non-linear relationships was computationally difficult at the time.
- Mid 1980s, classification and regression trees were developed, followed shortly by generalized additive models.
- 1980s: Neural networks gained popularity., and support vector machines arose in the 1990s.

- Though the term statistical learning is fairly new, many of the concepts that underlie the field were developed long ago.
- Early XIXth centurey: the method of least squares was developed, implementing the earliest form of what is now known as linear regression.
- Linear regression is used for predicting quantitative values.
- 1936: In order to predict qualitative values, linear discriminant analysis was proposed.
- 1940s: various authors put forth an alternative approach, logistic regression.
- Early 1970s: the term generalized linear model was developed to describe an entire class of statistical learning methods that include both linear and logistic regression as special cases.
- Late 1970s: more techniques for learning from data were available.
- However, they were almost exclusively linear methods be- cause fitting non-linear relationships was computationally difficult at the time.
- Mid 1980s, classification and regression trees were developed, followed shortly by generalized additive models.
- 1980s: Neural networks gained popularity., and support vector machines arose in the 1990s.
- 1990s: Support vector machines arose.

We thank Professors Hastie and Tibshirani for sharing their source files for the book 'An introduction to Statistical Learning'. We also thank professor Yang Ning for sharing the material which has inspired this one.