# STK-IN4300 Statistical Learning Methods in Data Science

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#### Outline of the lecture

Introduction

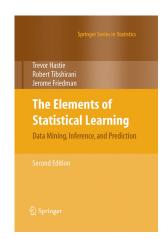
- Overview of supervised learning
  - Variable types and terminology
  - Two simple approaches to prediction
  - Statistical decision theory
  - Local methods in high dimensions
  - Data science, statistics, machine learning

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#### Introduction: Elements of Statistical Learning

This course is based on the book: "The Elements of Statistical Learning: Data Mining, Inference, and Prediction" by T. Hastie, R. Tibshirani and J. Friedman:

- reference book on modern statistical methods;
- free online version, https://web.stanford.edu/ ~hastie/ElemStatLearn/.



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Introduction: statistical learning

"We are drowning in information, but we starved from knowledge"
(J. Naisbitt)

- nowadays a huge quantity of data is continuously collected
   a lot of information is available;
- · we struggle with profitably using it;

The goal of statistical learning is to "get knowledge" from the data, so that the information can be used for prediction, identification, understanding, ...

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#### Introduction: email spam example

Goal: construct an automatic spam detector that block spam. Data: information on 4601 emails, in particular,

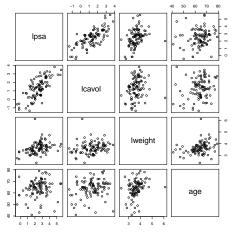
- whether was it spam (spam) or not (email);
- the relative frequencies of 57 of the most common words or punctuation marks.

word	george	you	your	hp	free	hpl	!	
spam	0.00	2.26	1.38	0.02	0.52	0.01	0.51	
email	1.27	1.27	0.44	0.90	0.07	0.43	0.11	

Possible rule: if (%george < 0.6) & (%you > 1.5) then spam else email

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#### Introduction: prostate cancer example



- data from Stamey et al. (1989);
- goal: predict the level of (log) prostate specific antigene (lpsa) from some clinical measures, such as log cancer volume (lcavol), log prostate weight (lweight), age (age), ...;
- possible rule:  $f(X) = 0.32 \ {\tt lcavol} + \\ 0.15 \ {\tt lweight} + 0.20 \ {\tt age}$

## Introduction: handwritten digit recognition

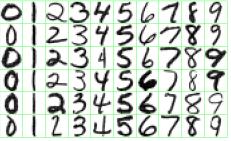


FIGURE 1.2. Examples of handwritten digits from U.S. postal envelopes.

- data: 16 x 16 matrix of pixel intensities;
- goal: identify the correct digit (0, ..., 9);
- the outcome consists of 10 classes.

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#### Introduction: other examples

## Examples (from the book):

- predict whether a patient, hospitalized due to a heart attack, will have a second heart attack, based on demographic, diet and clinical measurements for that patient;
- predict the price of a stock in 6 months from now, on the basis of company performance measures and economic data;
- identify the numbers in a handwritten ZIP code, from a digitized image;
- estimate the amount of glucose in the blood of a diabetic person, from the infrared absorption spectrum of that persons blood;
- identify the risk factors for prostate cancer, based on clinical and demographic.

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#### Introduction: framework

## In a typical scenario we have:

- an outcome Y (dependent variable, response)
  - quantitative (e.g., stock price, amount of glucose, ...);
  - categorical (e.g., heart attack/no heart attack)

#### that we want to predict based on

- a set of features  $X_1, X_2, \dots, X_p$  (independent variables, predictors)
  - examples: age, gender, income, . . .

## In practice,

- we have a training set, in which we observe the outcome and some features for a set of observations (e.g., persons);
- we use these data to construct a learner (i.e., a rule f(X)), which provides a prediction of the outcome  $(\hat{y})$  given specific values of the features.

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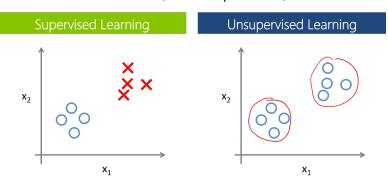
#### Introduction: supervised vs unsupervised learning

The scenario above is typical of a supervised learning problem:

• the outcome is measured in the training data, and it can be used to construct the learner f(X);

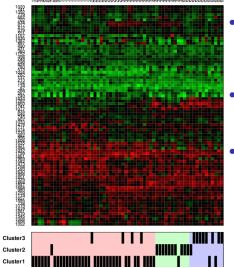
In other cases only the features are measured  $\rightarrow$  unsupervised learning problems:

• identification of clusters, data simplification, ...



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#### Introduction: gene expression example



- heatmap from De Bin & Risso (2011): 62 obs vs a subset of the original 2000 genes
  - p >> n problem;
- goal: group patients with similar genetic information (cluster);
- alternatives (if the outcome was also available):
  - classify patients with similar disease (classification);
  - predict the chance of getting a disease for a new patient (regression).

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#### Introduction: the high dimensional issue

Assume a training set  $\{(x_{i1},...,x_{ip},y_i), i=1,...,n\}$ , where n=100, p=2000;

- possible model:  $y_i = \beta_0 + \sum_{i=1}^p \beta_i x_{ij} + \varepsilon_i$ ;
- least squares estimate:  $\hat{\beta} = (X^T X)^{-1} X^T y$ .

#### Exercise:

- go together in groups of 3-4;
- learn the names of the others in the group;
- discuss problems with the least squares estimate in this case;
- discuss possible ways to proceed;

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#### Introduction: the high dimensional issue

Major issue:  $X^TX$  is not invertible, infinitely many solutions!

## Some possible directions:

- dimension reduction (reducing p to be smaller than n),
  - remove variables having low correlation with response;
  - more formal subset selections:
  - select a few "best" linear combinations of variables:
- shrinkage methods (adding constrain to  $\beta$ ),
  - ridge regression;
  - lasso (least absolute shrinkage and selection operator)
  - elastic net.

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#### Introduction: course information

- Course: mixture between theoretical and practical;
- evaluation: mandatory exercise(s) (practical) and written exam (theoretical);
- use of computer necessary;
- based on statistical package R:
  - suggestion: use R Studio (www.rstudio.com), available at all Linux computers at the Department of Mathematics;
  - encouragement: follow good R programming practices, for instance consult Google's R Style Guide.

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## Variable types and terminology

Variable types: quantitative (numerical), qualitative (categorical).

Naming convention for predicting tasks:

- quantitative response: regression;
- qualitative response: classification.

We start with the problem of taking two explanatory variables  $X_1$  and  $X_2$  and predicting a binary (two classes) response G:

- we illustrate two basic approaches:
  - linear model with least squares estimator;
  - k nearest neighbors;
- we consider both from a statistical decision theory point of view.

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## Two simple approaches to prediction: linear regression model

## The linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + \varepsilon$$
  
=  $X\beta + \varepsilon$ , where  $X = (1, x_1, \dots, x_p)$ ,

can be use to predict the outcome y given the values  $x_1, x_2, \dots, x_p$ , namely

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_p x_p$$

## Properties:

- easy interpretation;
- · easy computations involved;
- theoretical properties available;
- it works well in many situations.

#### Two simple approaches to prediction: least square

How do we fit the linear regression model to a training dataset?

- Most popular method: least square;
- estimate  $\beta$  by minimizing the residual sum of squares

$$RSS(\beta) = \sum_{i=1}^{N} (y_i - x_i^T \beta)^2 = (y - X\beta)^T (y - X\beta)$$

where X is a  $(N \times p)$  matrix and y a N-dimensional vector.

Differentiating w.r.t.  $\beta$ , we obtain the estimating equation

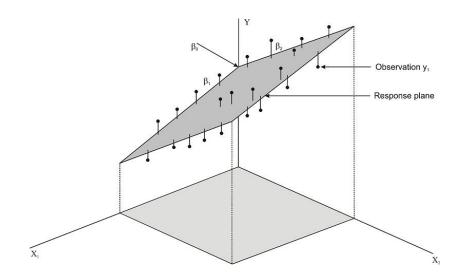
$$X^T(y - X\beta) = 0,$$

from which, when  $(X^TX)$  is non-singular, we obtain

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

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## Two simple approaches to prediction: least square



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## Two simple approaches to prediction: least square for binary response

Simulated data with two variables and two classes:

$$Y = \begin{cases} 1 & \text{orange} \\ 0 & \text{blue} \end{cases}$$

If  $Y \in \{0,1\}$  is treated as a numerical response

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2,$$

a prediction rule

$$\hat{G} = \begin{cases} 1 \text{ (orange)} & \text{if } \hat{Y} > 0.5\\ 0 \text{ (blue)} & \text{otherwise} \end{cases}$$

gives linear decision boundary  $\{x^T \hat{\beta} = 0.5\}$ 

- optimal under the assumption "one-Gaussian-per-class";
- is it better with nonlinear decision boundary?

## Two simple approaches to prediction: Nearest neighbor methods

A different approach consists in looking at the closest (in the input space) observations to x and, based on their output, form  $\hat{Y}(x)$ .

The k nearest neighbors prediction of x is the mean

$$\hat{Y}(x) = \frac{1}{k} \sum_{i: x_i \in N_k(x)} y_i,$$

where  $N_k(x)$  contains the k closest points to x.

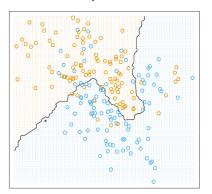
- less assumptions on f(x);
- we need to decide k;
- we need to define a metric (for now, consider the Euclidean distance).

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#### Two simple approaches to prediction: nearest neighbor methods

Use the same training data (simulated) as before:

$$Y = \begin{cases} 1 & \text{orange} \\ 0 & \text{blue} \end{cases}$$



Classify to orange, if there are mostly orange points in the neighborhood:

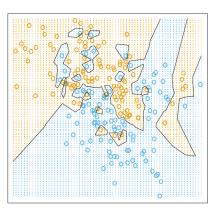
$$\hat{G} = \begin{cases} 1 \text{ (orange)} & \text{if } \hat{Y} > 0.5\\ 0 \text{ (blue)} & \text{otherwise} \end{cases}$$

- k = 15:
- flexible decision boundary;
- better performance than the linear regression case:
  - fewer training observations are missclassified;
  - is this a good criterion?

## Two simple approaches to prediction: nearest neighbor methods

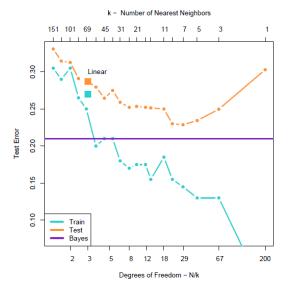
## Using the same data as before: Note:

$$Y = \begin{cases} 1 & \text{orange} \\ 0 & \text{blue} \end{cases}$$



- same approach, with k = 1;
- no training observations are missclassified!!!
- Is this a good solution?
  - the learner works greatly on the training set, but what its prediction ability? (remember this term: overfitting);
  - It would be preferable to evaluate the performance of the methods in an independent set of observations (test set);
- bias-variance trade-off.

## Two simple approaches to prediction: how many neighbors in KNN?



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#### Two simple approaches to prediction: alternatives

Most of the modern techniques are variants of these two simple procedures:

- kernel methods that weight data according to distance;
- in high dimension: more weight on some variables;
- local regression models;
- linear models of functions of *X*:
- projection pursuit and neural network.

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#### Statistical decision theory: theoretical framework

Statistical decision theory gives a mathematical framework for finding the optimal learner.

#### Let:

- $X \in \mathbb{R}^p$  be a p-dimensional random vector of inputs;
- $Y \in \mathbb{R}$  be a real value random response variable;
- p(X,Y) be their joint distribution;

Our goal is to find a function f(X) for predicting Y given X:

- we need a loss function L(Y, f(X)) for penalizing errors in f(X) when the truth is Y,
  - example: squared error loss,  $L(Y, f(X)) = (Y f(X))^2$ .

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#### Statistical decision theory: expected prediction error

Given p(X,Y), it is possible to derive the expected prediction error of f(X):

$$\mathsf{EPE}(f) = E\left[L(Y, f(X))\right] = \int_{x,y} L(y, f(x)) p(x, y) dx dy;$$

we have now a criterion for choosing a learner: find f which minimizes  $\mbox{EPE}(f).$ 

The aforementioned squared error loss,

$$L(Y, f(X)) = (Y - f(X))^{2},$$

is by far the most common and convenient loss function. Let us focus on it!

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#### Statistical decision theory: squared error loss

If 
$$L(Y, f(X)) = (Y - f(X))^2$$
, then

$$\begin{split} \mathsf{EPE}(f) = & E_{X,Y} \big[ (Y - f(X))^2 \big] \\ = & E_X E_{Y|X} \big[ (Y - f(X))^2 | X \big] \end{split}$$

It is then sufficient to minimize  $E_{Y|X}[(Y-f(X))^2|X]$  for each X:

$$f(x) = \operatorname{argmin}_c E_{Y|X}[(Y-c)^2|X=x],$$

which leads to

$$f(x) = E[Y|X = x],$$

i.e., the conditional expectation, also known as regression function.

Thus, by average squared error, the best prediction of Y at any point X=x is the conditional mean.

#### Statistical decision theory: estimation of optimal f

In practice, f(x) must be estimated.

## Linear regression:

- assumes a function linear in its arguments,  $f(x) \approx x^T \beta$ ;
- $\operatorname{argmin}_{\beta} E[(Y X^T \beta)^2] \rightarrow \beta = E[XX^T]^{-1} E[XY];$
- replacing the expectations by averages over the training data leads to  $\hat{\beta}$ .
- Note:
  - no conditioning on X;
  - we have used our knowledge on the functional relationship to pool over all values of *X* (model-based approach);
  - less rigid functional relationship may be considered, e.g.

$$f(x) \approx \sum_{j=1}^{p} f_j(x_j).$$

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#### Statistical decision theory: estimation of optimal f

## K nearest neighbors:

- uses directly f(x) = E[Y|X = x]:
- $\hat{f}(x_i) = \mathsf{Ave}(y_i)$  for observed  $x_i$ 's;
- normally there is at most one observation for each point  $x_i$ ;
- uses points in the neighborhood,

$$\hat{f}(x) = \mathsf{Ave}(y_i | x_i \in N_k(x))$$

- there are two approximations:
  - expectation is approximated by averaging over sample data;
  - conditioning on a point is relaxed to conditioning on a neighborhood.

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#### Statistical decision theory: estimation of optimal f

- assumption of k nearest neighbors: f(x) can be approximated by a locally constant function;
- for  $N \to \infty$ , all  $x_i \in N_k(x) \approx x$ ;
- for  $k \to \infty$ ,  $\hat{f}(x)$  is getting more stable;
- under mild regularity condition on p(X, Y),

$$\hat{f}(x) \to E[Y|X=x]$$
 for  $N, k \to \infty$  s.t.  $k/N \to 0$ 

- is this an universal solution?
  - small sample size;
  - curse of dimensionality (see later)

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#### Statistical decision theory: other loss function

- It is not necessary to implement the squared error loss function (L<sub>2</sub> loss function);
- a valid alternative is the  $L_1$  loss function:
  - the solution is the conditional median

$$\hat{f}(x) = \text{median}(Y|X = x)$$

- more robust estimates than those obtained with the conditional mean:
- the L<sub>1</sub> loss function has discontinuities in its derivatives → numerical difficulties.

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#### Statistical decision theory: other loss functions

## What happens with a categorical outcome G?

- similar concept, different loss function;
- $G \in \mathcal{G} = \{1, \dots, K\} \to \hat{G} \in \mathcal{G} = \{1, \dots, K\};$
- $L(G, \hat{G}) = L_{G, \hat{G}}$  a  $K \times K$  matrix, where K = |G|;
- each element of the matrix  $l_{ij}$  is the price to pay to missallocate category  $g_i$  as  $g_j$ 
  - ▶ all elements on the diagonal are 0;
  - often non-diagonal elements are 1 (zero-one loss function).

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#### Statistical decision theory: other loss functions

#### Mathematically:

$$EPE = E_{G,X}[L(G, \hat{G}(X))]$$

$$= E_X \left[ E_{G|X}[L(G, \hat{G}(X))] \right]$$

$$= E_X \left[ \sum_{k=1}^K L(g_k, \hat{G}(X)) \Pr(G = g_k | X = x) \right]$$

which is sufficient to be minimized pointwise, i.e,

$$\hat{G} = \operatorname{argmin}_{g \in \mathcal{G}} \sum_{k=1}^{K} L(g_k, g) \Pr(G = g_k | X = x).$$

When using the 0-1 loss function

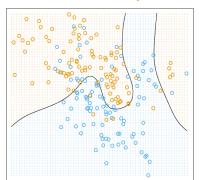
$$\begin{split} \hat{G} = & \operatorname{argmin}_{g \in \mathcal{G}} \sum_{k=1}^{K} \{1 - \mathbb{1}(G = g_k))\} \Pr(G = g_k | X = x) \\ = & \operatorname{argmin}_{g \in \mathcal{G}} \{1 - \Pr(G = g_k | X = x)\} \\ = & \operatorname{argmax}_{g \in \mathcal{G}} \Pr(G = g_k | X = x) \end{split}$$

#### Statistical decision theory: other loss functions

## Alternatively,

$$\hat{G}(x) = g_k \text{ if } P(G = g_k | X = x) = \max_{g \in \mathcal{G}} \Pr(G = g | X = x),$$

## also known as Bayes classifier.



- k nearest neighbor:
  - $\hat{G}(x) = \text{category with largest}$ frequency in k nearest samples;
  - approximation of this solution.
- regression:
  - $E[Y_k|X] = \Pr(G = g_k|X);$
  - also approximates the Bayes classifier.

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#### Local methods in high dimensions

## The two (extreme) methods seen so far:

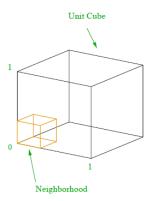
- linear model, stable but biased;
- k-nearest neighbor, less biased but less stable.

## For large set of training data:

- always possible to use k nearest neighbors?
- Breaks down in high dimensions → curse of dimensionality (Bellman, 1961).

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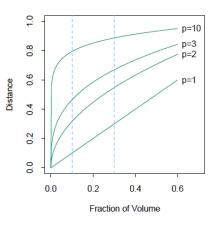
## Local methods in high dimensions: curse of dimensionality



- Assume  $X \sim \mathsf{Unif}[0,1]^p$ ;
- define  $e_p$  the expected length size of a hypercube containing a fraction r of input points;
- $e_p(r) = r^{1/p} (e^p = r \Leftrightarrow e = r^{1/p});$

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#### Local methods in high dimensions: curse of dimensionality



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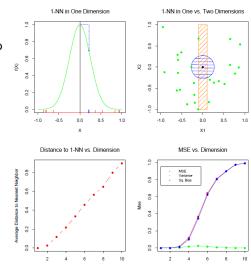
#### Local methods in high dimensions: curse of dimensionality

Assume  $Y = f(X) = e^{-8||X||^2}$  and use the 1-nearest neighbor to predict  $y_0$  at  $x_0 = 0$ , i.e.

 $\hat{y}_0 = y_i$  s.t.  $x_i$  nearest observed

$$\begin{aligned} \mathsf{MSE}(x_0) &= \\ &= E_{\mathcal{T}}[\hat{y}_0 - f(x_0)]^2 \\ &= E_{\mathcal{T}}[\hat{y}_0 - E_{\mathcal{T}}(\hat{y}_0)]^2 \\ &+ \left[ E_{\mathcal{T}}(\hat{y}_0) - f(x_0) \right]^2 \\ &= \mathsf{Var}(\hat{y}_0) + \mathsf{Bias}^2(\hat{y}_0) \end{aligned}$$

NB: we will see often this bias-variance decomposition!



#### Local methods in high dimensions: EPE in the linear model

- Assume now  $Y = X^T \beta + \varepsilon$
- we want to predict  $y_0 = x_0^T \beta + \varepsilon_0$  with  $x_0$  fixed
- $\hat{y}_0 = x_0^T \hat{\beta}$  where  $\hat{\beta} = (X^T X)^{-1} X^T y$

$$\begin{split} \mathsf{EPE}(x_0) &= E(y_0 - \hat{y}_0)^2 \\ &= E\left[ (y_0 - E[y_0|x_0] + E[y_0|x_0] - E[\hat{y}_0|x_0] + E[\hat{y}_0|x_0] - \hat{y}_0)^2 \right] \\ &= E(y_0 - E[y_0|x_0])^2 + (E[y_0|x_0] - E[\hat{y}_0|x_0])^2 \\ &\quad + E(\hat{y}_0 - E[\hat{y}_0|x_0])^2 \\ &= \mathsf{Var}(y_0|x_0) + \mathsf{Bias}^2(\hat{y}_0) + \mathsf{Var}(\hat{y}_0) \end{split}$$

True and assumed linear model

- Bias=0
- $Var(\hat{y}_0) = x_0^T E(X^T X)^{-1} x_0 \sigma^2$
- EPE $(x_0) = \sigma^2 + x_0^T E(X^T X)^{-1} x_0 \sigma^2$

#### Local methods in high dimensions: EPE in the linear model

- $\mathsf{EPE}(x_0) = \sigma^2 + x_0^T E(X^T X)^{-1} x_0 \sigma^2$
- If x's drawn from a random distribution with E(X) = 0,  $X^T X \to N \text{Cov}(X)$
- Assume also  $x_0$  drawn from same distribution:

$$\begin{split} E_{x_0} \left[ \mathsf{EPE}(x_0) \right] &\approx \! \sigma^2 + E_{x_0} \big[ x_0^T \mathsf{Cov}(X)^{-1} x_0 \big] N^{-1} \sigma^2 \\ &= \! \sigma^2 + N^{-1} \sigma^2 \mathsf{trace} \big[ \mathsf{Cov}(X)^{-1} E_{x_0} \big[ x_0 x_0^T \big] \big] \\ &= \! \sigma^2 + N^{-1} \sigma^2 \mathsf{trace} \big[ \mathsf{Cov}(X)^{-1} \mathsf{Cov}(x_0) \big] \\ &= \! \sigma^2 + N^{-1} \sigma^2 \mathsf{trace} \big[ I_p \big] \\ &= \! \sigma^2 + N^{-1} \sigma^2 p \end{split}$$

It increases linearly with p!

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Data science, statistics, machine learning: what is "data science"?

Carmichael & Marron (2018) stated: "Data science is the business of learning from data", immediately followed by "which is traditionally the business of statistics".

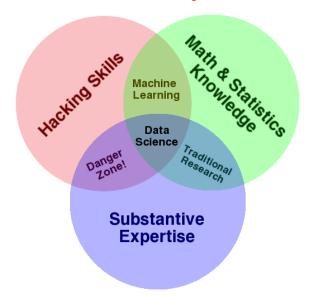
### What is your opinion?

- "data science is simply a rebranding of statistics"
   ("data science is statistics on a Mac", Bhardwaj, 2017)
- "data science is a subset of statistics"
   ("a data scientist is a statistician who lives in San Francisco",
   Bhardwai, 2017)
- "statistics is a subset of data scientist"
   ("statistics is the least important part of data science",
   Gelman, 2013)

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Data science, statistics, machine learning: what is "data science"?



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What about differences between statistics and machine learning?

- "Machine learning is essentially a form of applied statistics";
- "Machine learning is glorified statistics";
- "Machine learning is statistics scaled up to big data";
- "The short answer is that there is no difference":

(https://www.svds.com/machine-learning-vs-statistics)

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Let us be a little bit more provocative . . .

- "Machine learning is for Computer Science majors who couldn't pass a Statistics course";
- "Machine learning is Statistics minus any checking of models and assumptions";
- "I don't know what Machine Learning will look like in ten years, but whatever it is I'm sure Statisticians will be whining that they did it earlier and better".

(https://www.svds.com/machine-learning-vs-statistics)

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"The difference, as we see it, is not one of algorithms or practices but of *goals* and *strategies*.

Neither field is a subset of the other, and neither lays exclusive claim to a technique. They are like two pairs of old men sitting in a park playing two different board games. Both games use the same type of board and the same set of pieces, but each plays by different rules and has a different goal because the games are fundamentally different. Each pair looks at the other's board with bemusement and thinks they're not very good at the game."

"Both Statistics and Machine Learning create models from data, but for different purposes."

(https://www.svds.com/machine-learning-vs-statistics)

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#### **Statistics**

- "The goal of modeling is approximating and then understanding the data-generating process, with the goal of answering the question you actually care about."
- "The models provide the mathematical framework needed to make estimations and predictions."
- "The goal is to prepare every statistical analysis as if you were going to be an expert witness at a trial. [...] each choice made in the analysis must be defensible."
- "The analysis is the final product. Ideally, every step should be documented and supported, [...] each assumption of the model should be listed and checked, every diagnostic test run and its results reported."

(https://www.svds.com/machine-learning-vs-statistics)

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#### **Statistics**

 "In conclusion, the Statistician is concerned primarily with model validity, accurate estimation of model parameters, and inference from the model. However, prediction of unseen data points, a major concern of Machine Learning, is less of a concern to the statistician. Statisticians have the techniques to do prediction, but these are just special cases of inference in general."

(https://www.svds.com/machine-learning-vs-statistics)

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## **Machine Learning**

- "The predominant task is predictive modeling"
- "The model does not represent a belief about or a commitment to the data generation process. [...] the model is really only instrumental to its performance."
- "The proof of the model is in the test set."
- "freed from worrying about model assumptions or diagnostics.
   [...] are only a problem if they cause bad predictions."
- "freed from worrying about difficult cases where assumptions are violated, yet the model may work anyway."
- "The samples are chosen [...] from a static population, and are representative of that population. If the population changes [...] all bets are off."

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# Machine Learning

- "Because ML practitioners do not have to justify model choice or test assumptions, they are free to choose from among a much larger set of models. In essence, all ML techniques employ a single diagnostic test: the prediction performance on a holdout set."
- "As a typical example, consider random forests and boosted decision trees. The theory of how these work is well known and understood. [...] Neither has diagnostic tests nor assumptions about when they can and cannot be used. Both are "black box" models that produce nearly unintelligible classifiers. For these reasons, a Statistician would be reluctant to choose them. Yet they are surprisingly almost amazingly successful at prediction problems."

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# Machine Learning

- "In summary, both Statistics and Machine Learning contribute
  to Data Science but they have different goals and make
  different contributions. Though the methods and reasoning
  may overlap, the purposes rarely do. Calling Machine Learning
  applied Statistics is misleading, and does a disservice to both
  fields."
- "Computer scientists are taught to design real-world algorithms that will be used as part of software packages, while statisticians are trained to provide the mathematical foundation for scientific research. [...] Putting the two groups together into a common data science team (while often adding individuals trained in other scientific fields) can create a very interesting team dynamic."

(https://www.svds.com/machine-learning-vs-statistics)

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