Lecture 001

Statistical learning: Foundations

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January 2022

Admin

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Today

In-class

- *Course website:* https://github.com/edrubin/EC524W22/
- *Resources*
  - RStudio cheatsheets, books, and tutorials
  - UO library
  - See course page for more...
- Formalizing statistical learning, notation, goals (and problems)

Eugene R Users Retweeted

Ryann Crowley
@ryann_crowley

Interested in an intro to #MachineLeaning, sharing info, developing an ML community, or curious about ML opportunities in Eugene? Come meet/learn at "Machine learning for the web" hosted by the Eugene Web Developers @EugeneRUsers @uodatasci @WiMLDS_PDX

Tweet; h/t: Grant McDermott

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Upcoming

Readings

- *Today*
  - *ISL* Ch. 1–2
  - Prediction Policy Problems by Kleinberg *et al.* (2015)
- *Next*
  - *ISL* Ch. 3–4

Problem set Soon.

Statistical learning

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- **Regression trees** extend *classification trees* to numerical outcomes (random forests extend, as well).
- **K-means clustering** partitions observations into K groups (clusters) based upon a set of variables.

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   that accurately describes $\mathbf{y}$ given some values of $\mathbf{x}_1, \ldots, x_p$.

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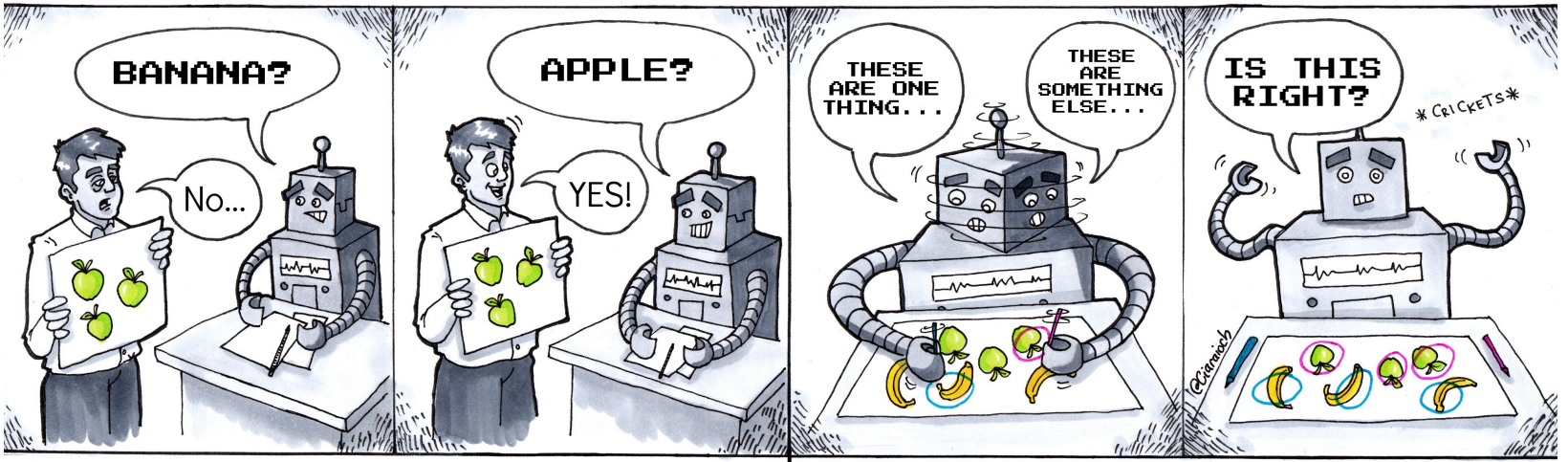
2. **Unsupervised learning** learns relationships and structure using only **inputs** ($x_1, \ldots, x_p$) without any *supervising* output—letting the data "speak for itself."

Semi-supervised learning falls somewhere between these supervised and unsupervised learning—generally applied to supervised tasks when labeled **outputs** are incomplete.



Supervised Learning

Unsupervised Learning

Source

Statistical learning

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1. **Classification tasks** for which the values of $\mathbf{y}$ are discrete categories
   E.g., race, sex, loan default, hazard, disease, flight status

2. **Regression tasks** in which $\mathbf{y}$ takes on continuous, numeric values.
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$Note_1$ The use of *regression* differs from our use of *linear regression*.

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$Note_1$ The use of *regression* differs from our use of *linear regression*.

$Note_2$ Don't get tricked: Not all numbers represent continuous, numerical values—*e.g.*, zip codes, industry codes, social security numbers.[†]

† Q Where would you put responses to 5-item Likert scales?

Statistical learning

Why *Learning*?

Q What puts the "learning" in statistical/machine learning?

Statistical learning

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Q What puts the "learning" in statistical/machine learning?

A Most learning models/algorithms will **tune model parameters** based upon the observed dataset—learning from the data.

Notation

Our class will typically follow the notation and definitions of *ISL*.

Notation

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n gives the number of observations

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$$\mathbf{X} = \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,p} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,p} \end{bmatrix}$$

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Applied to R:

- `dim(x_df)` = n p
- `nrow(x_df)` = n; `ncol(x_df)` = p
- `x_df[1,]` ($i = 1$); `x_df[,1]` ($j = 1$)

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and our full dataset is composed of $\left\{ (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n) \right\}$.

Back to the problem of (supervised) statistical learning...

Statistical learning

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You'll have to wait on any real/specific answers...

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Learning from $\hat{f}$

There are two main reasons we want to learn about f

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Statistical learning

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   our *black-box setting* where we care less about f than $\hat{\mathbf{y}}$.†

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Similarly, in causal-inference settings, we don't particulary care about $\hat{\mathbf{y}}$.

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Prediction errors

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Note As its name implies, you can't get rid of *irreducible* error—but we can try to get rid of *reducible* errors.

Prediction errors

Why we're stuck with *irreducible* error

$$
\begin{aligned}
E\left[\{\mathbf{y} - \hat{\mathbf{y}}\}^2\right] &= E\left[\left\{f(\mathbf{X}) + \varepsilon - \hat{f}\,(\mathbf{X})\right\}^2\right] \\
&= \underbrace{\left[f(\mathbf{X}) - \hat{f}\,(\mathbf{X})\right]^2}_{\text{Reducible}} + \underbrace{\mathrm{Var}(\varepsilon)}_{\text{Irreducible}}
\end{aligned}
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In less math:

- If ε exists, then $\mathbf{X}$ cannot perfectly explain $\mathbf{y}$.
- So even if $\hat{f} = f$, we still have irreducible error.

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Thus, to form our **best predictors**, we will **minimize reducible error**.

Statistical learning

Which type of $\hat{f}$?

Once you have your inputs ($\mathbf{X}$) and output ($\mathbf{y}$) data, you still need to decide how parametric your $\hat{f}$ should be.[†]

† I'm saying "how parametric" b/c some methods are much more parametric than others.

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Once you have your inputs ($\mathbf{X}$) and output ($\mathbf{y}$) data, you still need to decide how parametric your $\hat{f}$ should be.[†]

Parametric methods assume a function typically involve two steps

1. Select a functional form (shape) to represent f
2. Train your selected model on your data $\mathbf{y}$ and $\mathbf{X}$.

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Parametric methods assume a function typically involve two steps

1. Select a functional form (shape) to represent f
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Non-parametric methods avoid explicit assumption about the shape of f. Attempt to flexibly fit the data, while trying to avoid overfitting.

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Which type of $\hat{f}$?

Methods' parametric assumptions come with tradeoffs.

Parametric methods

+ Simpler to estimate and interpret.
– If assumed functional form is bad, model performance will suffer.

Non-parametric methods

+ Fewer assumptions. More flexibility.
– Lower interpretability. Susceptible to overfitting. Want lots of data.

Example: Let's start with a pretty funky, nonlinear function.

Truth: The (nonlinear) $f(\mathbf{X})$ that we hope to recover.

The sample: $n = 70$ randomly drawn observations for $\mathbf{y} = f(\mathbf{x}_1, \mathbf{x}_2) + \varepsilon$

Estimated linear-regression model: $\hat{\mathbf{y}} = \hat{\beta}_0 + \hat{\beta}_1 \mathbf{x}_1 + \hat{\beta}_2 \mathbf{x}_2 + \hat{\beta}_3 \mathbf{x}_1 \mathbf{x}_2$

Prediction error from our fitted linear regression model

k-nearest neighbors (kNN) using k=5 (a *non-parametric* method)

k-nearest neighbors (kNN) using k=10 (notice increased smoothness)

k-nearest neighbors (kNN) using k=1 (notice decreased smoothness)

Prediction error from our fitted kNN (k=5) model

Prediction error from our fitted kNN (k=10) model

Prediction error from our fitted kNN (k=1) model

Recall **Prediction error** from our fitted linear regression model

Model accuracy

Questions

1. Which of the methods was the most flexible? Inflexible?

2. Why do you think kNN with k=1 had such low prediction error?

3. How could we (better) assess model/predictive performance?

4. Why would we ever want to choose a less flexible model?

Model accuracy

Measurement

You probably will not be surprised to know that there is no one-size-fits-all solution in statistical learning.

Q How do we choose between competing models?

Model accuracy

Measurement

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Q How do we choose between competing models?

A We're a few steps away, but before we do anything, we need a way to **define model performance**.

Model accuracy

Subtlety

Defining performance can actually be quite tricky...

Regression setting, 1 Which do you prefer?

1. Lots of little errors and a few really large errors.
2. Medium-sized errors for everyone.

Regression setting, 2 Is a 1-unit error (*e.g.*, $1,000) equally bad for everyone?

Model accuracy

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Classification setting, 1 Which is worse?

1. False positive (*e.g.*, incorrectly diagnosing cancer)
2. False negative (*e.g.*, missing cancer)

Classification setting, 2 Which is more important?

1. True positive (*e.g.*, correct diagnosis of cancer)
2. True negative (*e.g.*, correct diagnosis of "no cancer")

Model accuracy

MSE

Mean squared error (MSE) is the most common[†] way to measure model performance in a regression setting.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left[y_i - \hat{f}\left(x_i\right)\right]^2$$

Recall: $y_i - \hat{f}\left(x_i\right) = y_i - \hat{y}_i$ is our prediction error.

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Two notes about MSE

1. MSE will be (relatively) very small when **prediction error** is nearly zero.
2. MSE **penalizes** big errors more than little errors (the squared part).

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Model accuracy

Training or testing?

Low MSE (accurate performance) on the data that trained the model isn't actually impressive—maybe the model is just overfitting our data.[†]

What we want: How well does the model perform **on data it has never seen**?

† Recall the kNN performance for k=1.

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What we want: How well does the model perform **on data it has never seen**?

This introduces an important distinction:

1. **Training data**: The observations (y_i, x_i) used to **train** our model $\hat{f}$.
2. **Testing data**: The observations (y_0, x_0) that our model has yet to see—and which we can use to evaluate the performance of $\hat{f}$.

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Real goal: Low test-sample MSE (not the training MSE from before).

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Next time: model performance, the variance-bias tradeoff, and kNN

Sources

These notes draw upon

- An Introduction to Statistical Learning (*ISL*)
  James, Witten, Hastie, and Tibshirani

- Python Data Science Handbook
  Jake VanderPlas

I pulled the comic from Twitter.

Table of contents