

# Introduction

Ryan Miller

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  - ▶ Computer programs rely on written rules, machine learning develops rules by finding patterns in examples
- ▶ How is machine learning similar/different from statistics?
  - ▶ Statistics focuses on inference about a population using a sample, machine learning seeks generalizable predictive patterns

# What is Machine Learning?

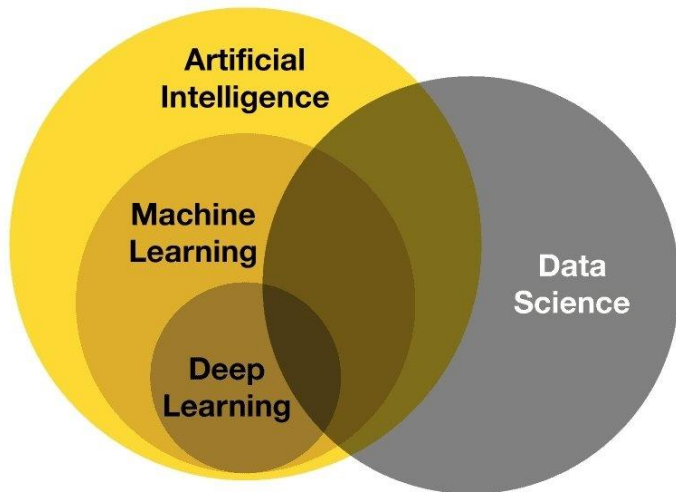
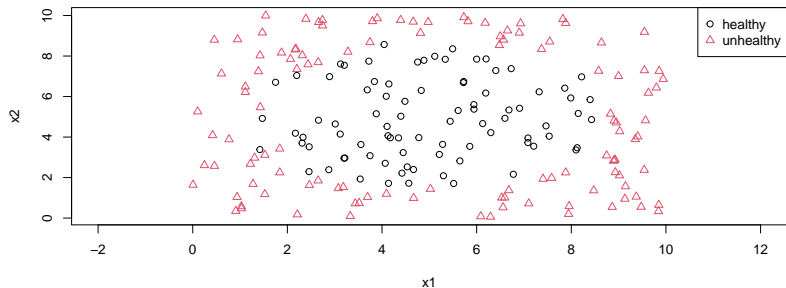


Image credit: BBN Times



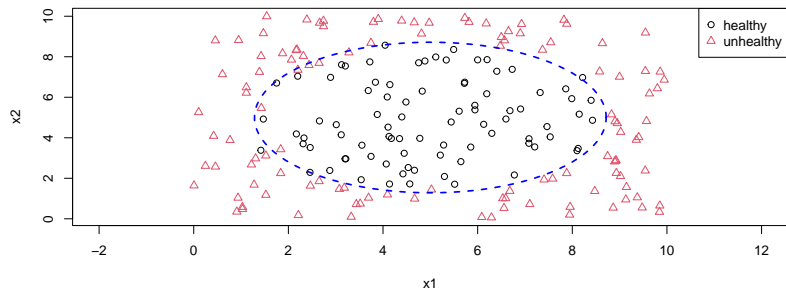
## Example

Consider two predictors,  $x_1$  and  $x_2$ , and an outcome  $y$  of “healthy” or “unhealthy”. Can these predictors be used to accurately *classify* an observation?



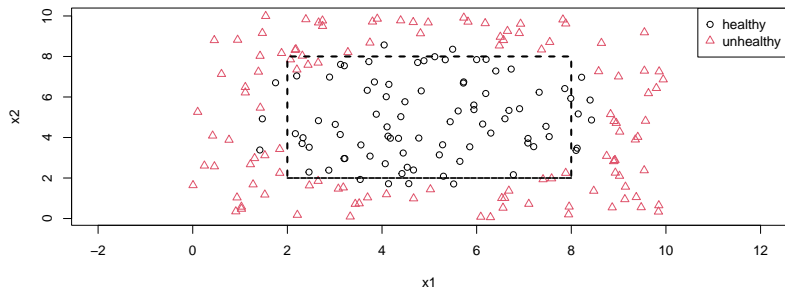
## Example (cont.)

Yes! In this example, the true relationship between predictors and the outcome is given by the blue ellipse



# Learning?

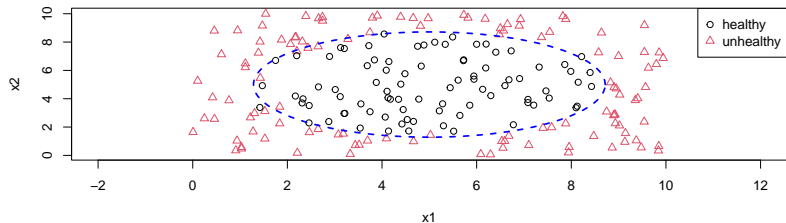
As a human, you might observe that the healthy data-points tend to fall between 2 and 8 in  $x_1$  and  $x_2$ , so you might propose the following *classification model*:



This simple model correctly classifies 178 of 200 data-points.

## Reducible vs. Irreducible Error

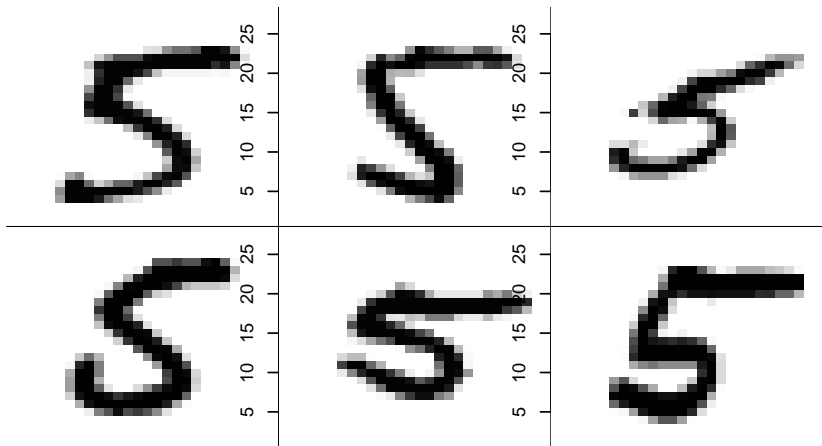
Let's revisit the true relationship between  $x_1$ ,  $x_2$ , and  $y$ . Notice that some “healthy” data-points are outside the ellipse, and some “unhealthy” ones are inside it:



- ▶ The misclassification of these examples is known as the **irreducible error** (sometimes called “Bayes error”)
  - ▶ Even the *best possible model* still cannot perfectly predict every outcome

# Irreducible Error in Real Life

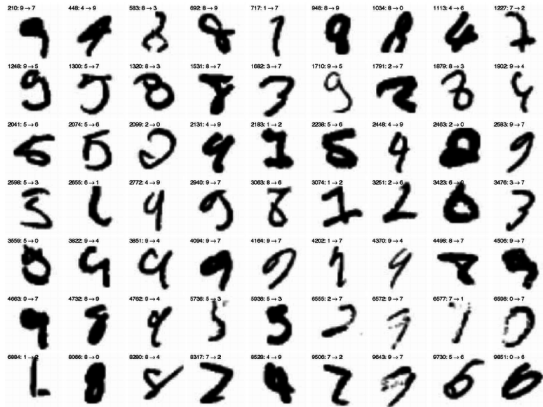
Is a digit a “5” or something else?



How might the concept of irreducible error manifest in this application?

# Irreducible Error in Real Life

We could know the exact “rules” used to make a “5”, but it’s possible we encounter examples of “5” that look more like a “6”.



Even state of the art classifiers (which approach the irreducible error rate) misclassify  $\sim 0.5\%$  of handwritten digits (source)

# Irreducible Error in Real Life

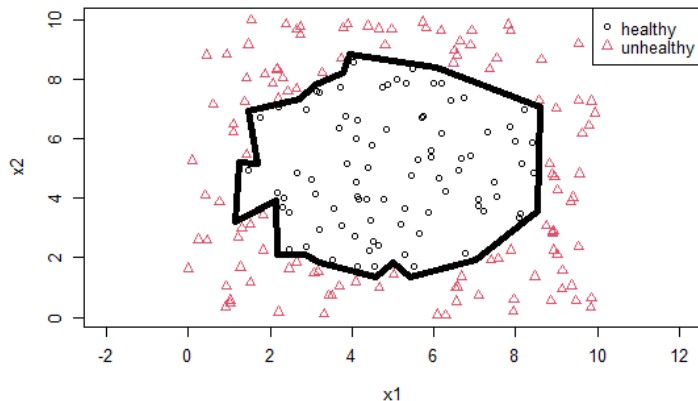
Irreducible error will always exist, the important question is “how much?” Consider the following scenarios:

- ▶ Classifying examples of “5” handwritten by a doctor
- ▶ Classifying examples of “5” created by a laser printer

While the precise amount of irreducible error in a machine learning problem is generally unknown, we often have a sense of what it might be.

## Reducible Error

The primary goal of machine learning is to *learn rules* that minimize *reducible error*. Consider the following classifier:



Has this classifier reduced the error rate to zero?



## Training vs. Testing Splits

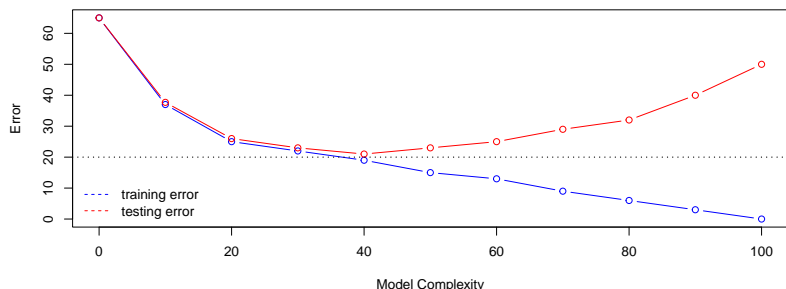
- ▶ We generally aren't interested in the error rate for the *observed examples*
  - ▶ Instead, we'd like to minimize reducible error on *new examples* that our model *hasn't yet seen*

# Training vs. Testing Splits

- ▶ We generally aren't interested in the error rate for the *observed examples*
  - ▶ Instead, we'd like to minimize reducible error on *new examples* that our model *hasn't yet seen*
- ▶ Standard procedure is to divide the available data into **training** and **testing** sets
  - ▶ The training set is used to learn a collection of rules
  - ▶ The testing set is used to evaluate how well these rules perform on data that hasn't been seen by the learner

# Training, Testing, and Error

Consider a hypothetical example with an irreducible error of “20 units”:



Training error can always be reduced by increasing the model complexity (ie: learning more rules), but testing error will never drop below the irreducible error (probabilistically speaking, it might for a single test set)

# Bias vs. Variance

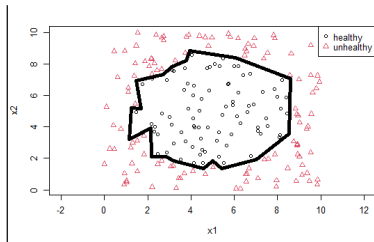
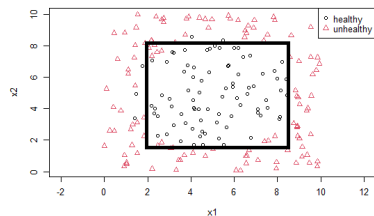
Reducible error can arise in one of two ways: **bias** or **variance**

- ▶ **Bias** is when a learner lacks the structural flexibility to detect aspects of the true relationship between the predictors and the outcome
- ▶ **Variance** is when a learner is overly sensitive to chance artifacts present in the data (ie: the manifestations of irreducible error)

Poor performance due to high bias is called *underfitting*, while poor performance due to high variance is called *overfitting*

# Bias vs. Variance

How would you compare the bias and variance of the following learners (a rectangle vs. an n-dimensional polygon)?



## Defining Error

- ▶ So far we've focused on classifying a binary categorical outcome, a scenario where *classification accuracy* provides a natural framework for understanding a method's error
  - ▶ We'll talk about more sophisticated ways to evaluate error for categorical outcomes next week
- ▶ What if our goal is to predict a numeric outcome?

## Defining Error

For a numeric outcome, it's most natural to measure error by summarizing the distances between predicted and observed outcomes:

- ▶ **Root Mean Squared Error:**  $RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$
- ▶ **Mean Absolute Error:**  $MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$

In each definition,  $y_i$  is the observed outcome for the  $i^{th}$  example (data-point) and  $\hat{y}_i$  is the predicted outcome for that example.

# Classification vs. Regression

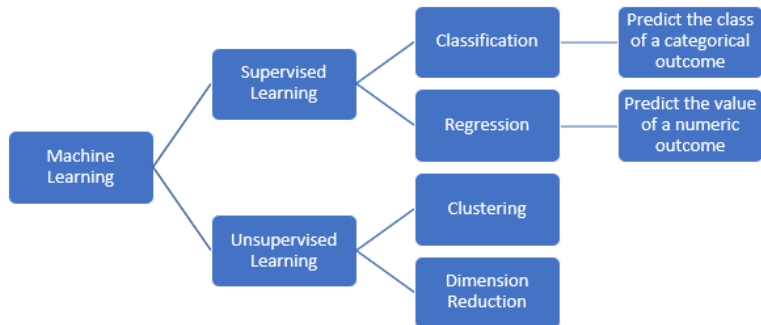
- ▶ Machine learning applications involving a *numeric outcome* are called **regression tasks**
  - ▶ Applications involving a *categorical outcome* are called **classification tasks**
- ▶ We define error differently for each type of task
  - ▶ The bias-variance trade-off and irreducible error still apply to both scenarios



# Machine Learning without an Outcome?

- ▶ For most of this semester, we'll focus on machine learning tasks involving a pre-selected or derived outcome
  - ▶ These are known as **supervised learning** tasks
- ▶ Other learning tasks, such as clustering or dimension reduction, can be achieved without designating an outcome
  - ▶ These are known as **unsupervised learning** tasks

# Overview



## Things to know for Thursday's quiz

1. Definitions and examples of reducible vs. irreducible error
2. The bias-variance trade-off
3. The reason for creating a training and testing split
4. Definitions and differences between classification and regression