

MY474: Applied Machine Learning for Social Science

Lecture 2: Generalization, Inference, Prediction, and Causality

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Concepts

1. To Explain vs. Predict
2. Generalization
3. Bias Variance Tradeoff
4. Measuring Error
5. Discussion Questions for Q&A Session

To explain or predict (β vs. \hat{y})

Glossary of Terms

Machine learning	Statistics
network, graphs	model
weights	parameters
learning	fitting
generalization	test set performance
supervised learning	regression/classification
unsupervised learning	density estimation, clustering
large grant = \$1,000,000	large grant = \$50,000
nice place to have a meeting: Snowbird, Utah, French Alps	nice place to have a meeting: Las Vegas in August

Source: <http://bit.ly/statvsml>

Social Science vs. Machine Learning?

Machine learning

\hat{y}
Predict

Social Science

vs.
and
 $\hat{\beta}$
Explain

Important to view **prediction** and **explanation** as
compliments, not substitutes

Source: Mullainathan & Spiess, JEP 2017

Why Machine Learning

- ▶ Prediction is often useful in its own right
 - e.g., *forecasting economic outcomes, quantifying risk*
- ▶ Prediction can help fill in missing data
 - e.g., *inferring online demographics*
- ▶ Prediction can aid in causal inference
 - e.g., *matching, instrumental variables, heterogenous effects*
- ▶ Predictive models can provide benchmarks for causal theories
 - e.g., *gap in performance indicates work to be done*

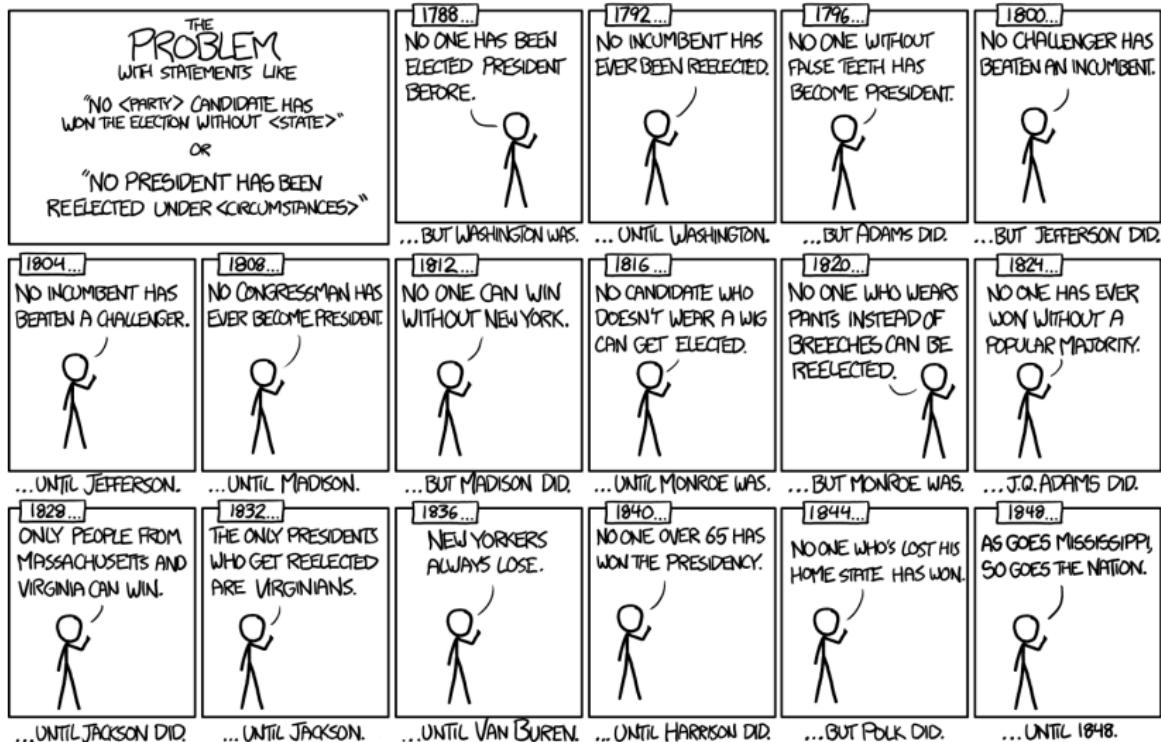
Source: Mullainathan & Spiess, JEP 2017

To explain or predict (β vs. \hat{y})

- ▶ Can use the same model to explain and predict, but the approaches are distinct!
- ▶ Explain
 - ▶ Causality comes from theory, usually not the model itself
 - ▶ Inference, parameter estimates help us explain causal relationships
 - ▶ Simpler model, variables that are statistically significant, not collinear
 - ▶ Model should be close to “true model”
 - ▶ Look at p-values
- ▶ Predict
 - ▶ Predict future outcomes given past observations
 - ▶ Evaluated based on generalization error
 - ▶ Collinearity does not matter
 - ▶ Model does not have to resemble a “true model”

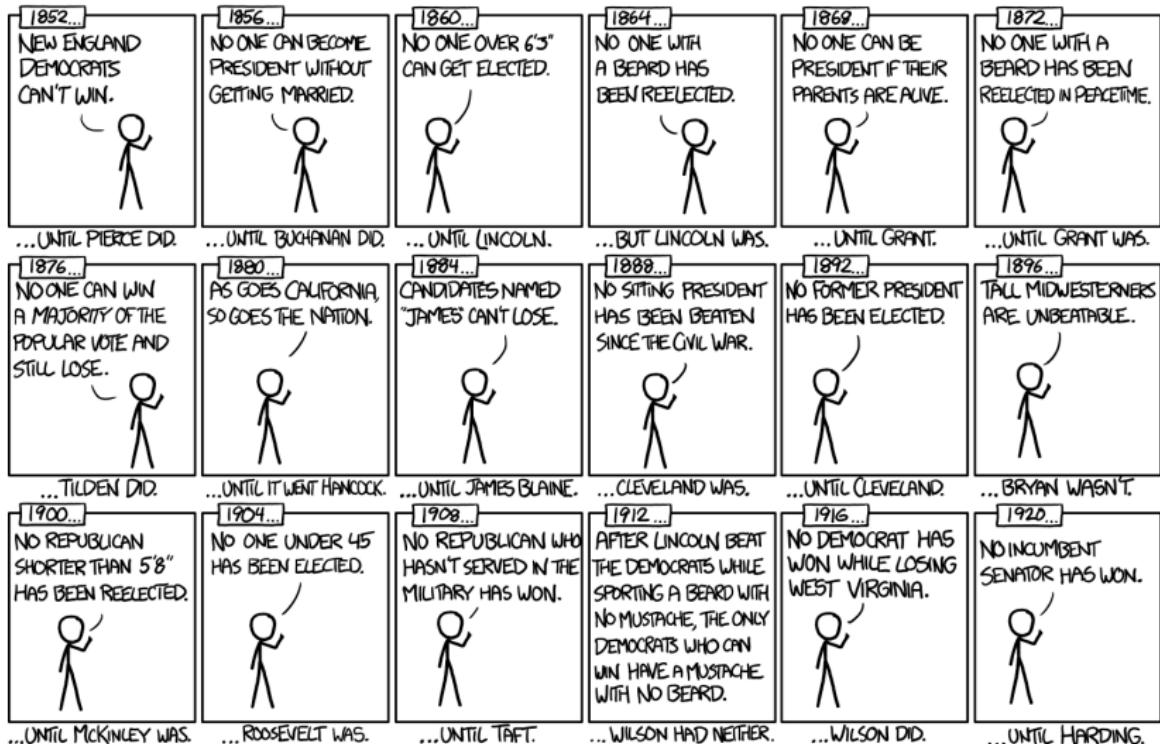
Generalization

Failing to Generalize: Overfitting



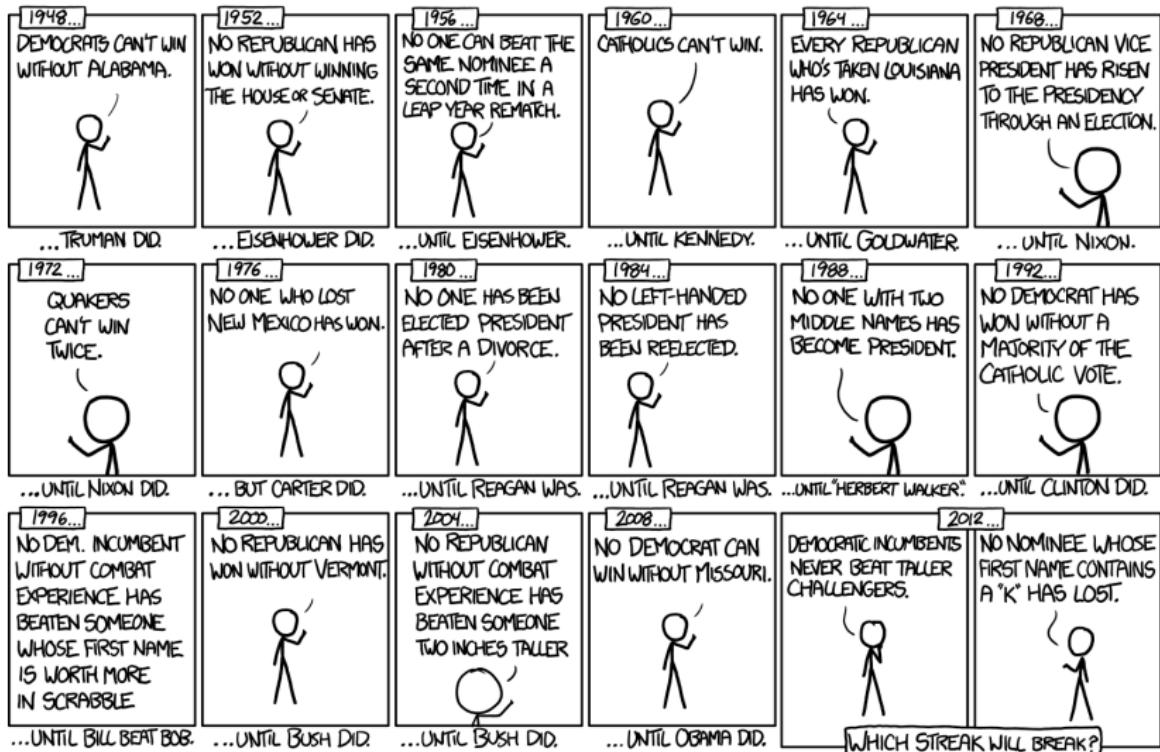
Source: xkcd.com

Failing to Generalize: Overfitting



Source: xkcd.com

Failing to Generalize: Overfitting



Generalization

- ▶ Recall that our goal in supervised learning is to approximate an unknown function $f(x)$ from data \mathcal{D} .
 - ▶ The approximation is called (equivalently) \hat{y} , $g(x)$, or $\hat{f}(x)$
 - ▶ We ideally want to choose a $g(x) \in \mathcal{H}$ that is close to y
- ▶ But there are many possible $h(x) \in \mathcal{H}$ that will do a good job. Which one do we choose for $g(x)$?
- ▶ A good approximation of $f(x)$ should **generalize** to new, unseen data
 - ▶ But what if we can't collect new data? How do we measure how well $g(x)$ generalizes?

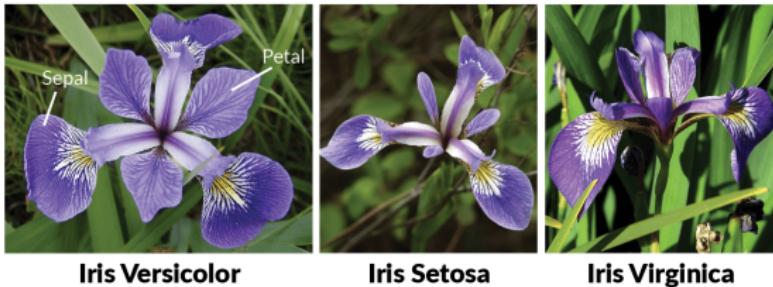
Training vs. test error

- ▶ Instead of collecting new data, we can divide the data into a **training** and **test** set
- ▶ We use the **training set** to learn $g(x)$ and the **test set** to measure how $g(x)$ generalizes to unseen data.
- ▶ **Training error** compares y to $g(x)$ using the training set
 - ▶ Tends to be optimistic because $g(x)$ was learned from the same data used to calculate the error
- ▶ **Test error** compares y to $g(x)$ using the test set
 - ▶ Better estimates how $g(x)$ generalizes to new data; error is calculated using data not used to learn $g(x)$

Two simple measures of error

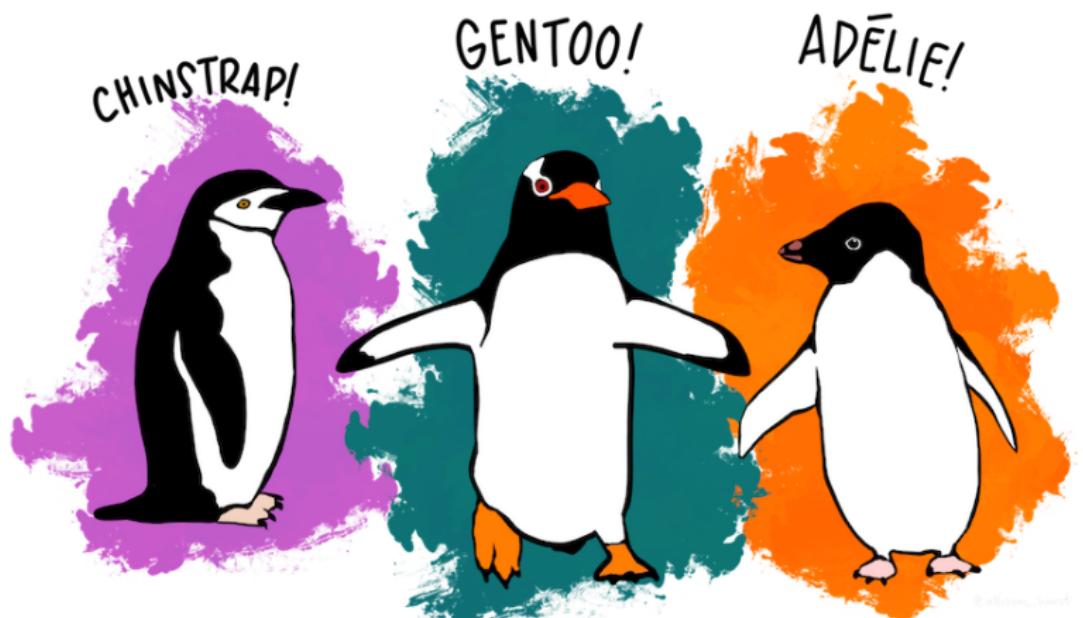
- ▶ **Mean-squared prediction error:** a measure used to evaluate performance of $g(x)$ for regression problems
 - ▶ Training error: $MSE_{Tr} = \text{Ave}_{i \in Tr} [y_i - g(x_i)]^2$ (biased when overfitting)
 - ▶ Test error: $MSE_{Te} = \text{Ave}_{i \in Te} [y_i - g(x_i)]^2$ (mitigates bias by using **out of sample** data)
- ▶ **Misclassification error rate:** a measure used to evaluate performance of $g(x)$ for classification problems
 - ▶ Training error: $Err_{Tr} = \text{Ave}_{i \in Tr} I[y_i \neq g(x_i)]$
 - ▶ Test error: $Err_{Te} = \text{Ave}_{i \in Te} I[y_i \neq g(x_i)]$

Example: Fisher's Iris Data



- ▶ While making these slides I learned that that this dataset was originally published in *The Annals of Eugenics*.
- ▶ Fisher's contributions to statistics are numerous, but he was also a prominent eugenicist and strong proponent of racist policies.
- ▶ Read more about the racist foundations of Fisher's scholarship and the field of Statistics [here](#).
- ▶ Rather than use Fisher's dataset, I found a substitute: penguins!

Example: Classifying Penguins

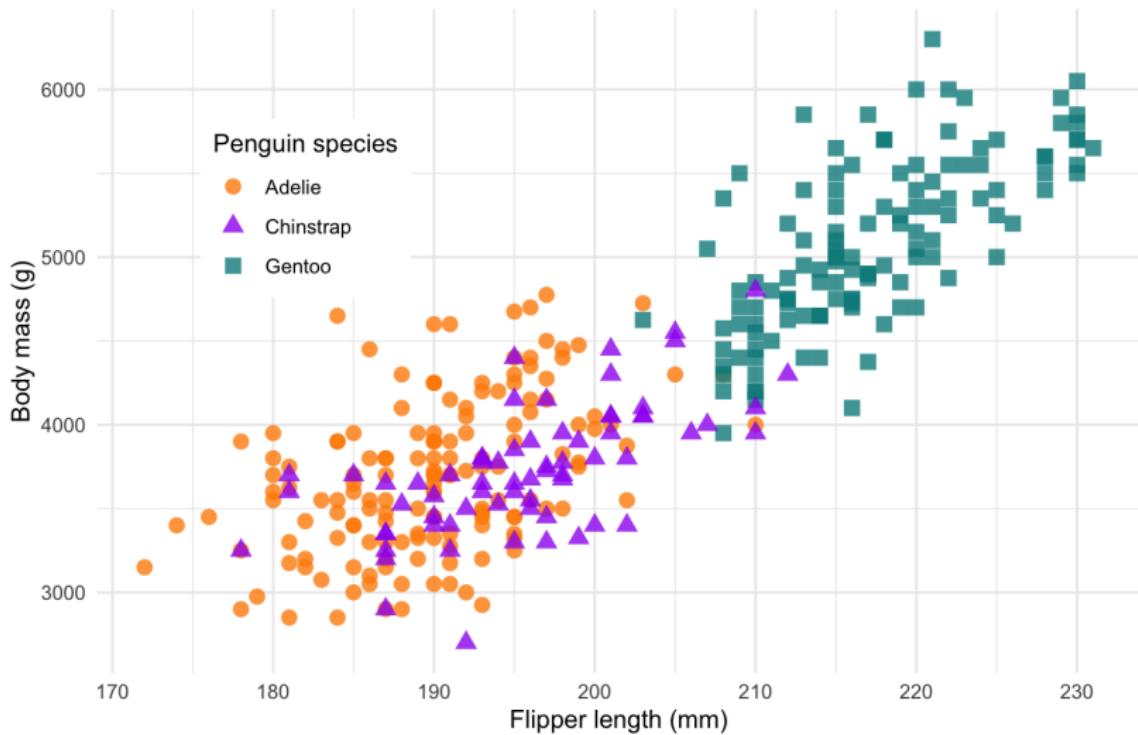


Artwork by @allison_horst

Example: Classifying Penguins

Penguin size, Palmer Station LTER

Flipper length and body mass for Adelie, Chinstrap, and Gentoo Penguins



Penguin Data from the Palmer Station in Antarctica

ID	Variable	Description
1	species	penguin species ("adeline," "chinstrap," and "gentoo")
2	island	island ("biscoe," "dream," or "torgersen")
3	bill_length_mm	bill length in millimeters
4	bill_depth_mm	bill depth in millimeters
5	flipper_length_mm	flipper length in millimeters
6	body_mass_g	body mass in grams
7	sex	penguin sex ("female," "male")
8	year	the study year (2007, 2008, or 2009)

Penguin Data

```
# remotes::install_github("allisonhorst/palmerpenguins")
library(palmerpenguins)
data(penguins)
table(penguins$species)

##
##      Adelie  Chinstrap    Gentoo
##          152         68        124

cols <- c(1,5,6)
penguins <- penguins[complete.cases(penguins), cols]
nrow(penguins)

## [1] 333
```

Split into Training and Test Sets

```
n_test <- floor(nrow(penguins) * 0.3)
idx <- sample(1:nrow(penguins), n_test)
# ?sample to learn about this function
head(idx)
```

```
## [1] 324 167 129 299 270 187
```

```
te <- penguins[idx,]
tr <- penguins[-idx,]
nrow(te)
```

```
## [1] 99
```

```
nrow(tr)
```

```
## [1] 234
```

Multinomial Logistic Regression

```
# install.packages("VGAM")
library(VGAM)

logit = vglm(species ~ ., family=multinomial, tr)
prob <- predict(logit, tr, type="response")
pred <- apply(prob, 1, which.max)
pred[which(pred=="1")] <- levels(tr$species)[1]
pred[which(pred=="2")] <- levels(tr$species)[2]
pred[which(pred=="3")] <- levels(tr$species)[3]
```

Logit Confusion Matrix (Train)

```
table(tr$species, pred)
```

```
##           pred
##             Adelie Chinstrap Gentoo
##   Adelie      85       12       0
##   Chinstrap    29       15       4
##   Gentoo       1        1      87
```

Logit Training Error

```
ade_tr <- which(tr$species == 'Adelie')
chi_tr <- which(tr$species == 'Chinstrap')
gen_tr <- which(tr$species == 'Gentoo')

mean(pred[ade_tr] == 'Adelie')
## [1] 0.8762887

mean(pred[chi_tr] == 'Chinstrap')
## [1] 0.3125

mean(pred[gen_tr] == 'Gentoo')
## [1] 0.9775281
```

Logit Confusion Matrix (Test)

```
prob <- predict(logit, te, type="response")
pred <- apply(prob, 1, which.max)
pred[which(pred=="1")] <- levels(te$species) [1]
pred[which(pred=="2")] <- levels(te$species) [2]
pred[which(pred=="3")] <- levels(te$species) [3]
table(te$species, pred)
```

```
##          pred
##          Adelie Chinstrap Gentoo
##    Adelie      41        7       1
##    Chinstrap     8       12       0
##    Gentoo       0        1      29
```

Logit Test Error

```
ade_te <- which(te$species == 'Adelie')
chi_te <- which(te$species == 'Chinstrap')
gen_te <- which(te$species == 'Gentoo')

mean(pred[ade_te] == 'Adelie')
## [1] 0.8367347

mean(pred[chi_te] == 'Chinstrap')
## [1] 0.6

mean(pred[gen_te] == 'Gentoo')
## [1] 0.9666667
```

K-Nearest Neighbors

```
#install.packages('class')
library(class)

tr_sc <- scale(tr[,-c(1)])
te_sc <- scale(te[,-c(1)])

pred_3 <- knn(tr_sc, tr_sc, tr$species, k=3)
pred_100 <- knn(tr_sc, tr_sc, tr$species, k=100)
```

KNN Confustion Matrices (Train)

```
table(tr$species, pred_3)
```

```
##          pred_3
##          Adelie Chinstrap Gentoo
##  Adelie      89       7      1
##  Chinstrap    21      24      3
##  Gentoo       0       2     87
```

```
table(tr$species, pred_100)
```

```
##          pred_100
##          Adelie Chinstrap Gentoo
##  Adelie      95       0      2
##  Chinstrap    42       0      6
##  Gentoo       1       0     88
```

KNN ($k = 3$) Training Error

```
mean(pred_3[ade_tr] == 'Adelie')
```

```
## [1] 0.9175258
```

```
mean(pred_3[chi_tr] == 'Chinstrap')
```

```
## [1] 0.5
```

```
mean(pred_3[gen_tr] == 'Gentoo')
```

```
## [1] 0.9775281
```

KNN ($k = 100$) Training Error

```
mean(pred_100[ade_tr] == 'Adelie')  
## [1] 0.9793814  
  
mean(pred_100[chi_tr] == 'Chinstrap')  
## [1] 0  
  
mean(pred_100[gen_tr] == 'Gentoo')  
## [1] 0.988764
```

KNN Confustion Matrices (Test)

```
pred_3 <- knn(tr_sc, te_sc, tr$species, k=3)
pred_100 <- knn(tr_sc, te_sc, tr$species, k=100)
table(te$species, pred_3)
```

```
##          pred_3
##          Adelie Chinstrap Gentoo
##  Adelie      37       10       2
##  Chinstrap    9        11       0
##  Gentoo       0        0      30
```

```
table(te$species, pred_100)
```

```
##          pred_100
##          Adelie Chinstrap Gentoo
##  Adelie      46       0       3
##  Chinstrap    19       0       1
##  Gentoo       0        0      30
```

KNN ($k = 3$) Test Error

```
mean(pred_3[ade_te] == 'Adelie')  
## [1] 0.755102  
  
mean(pred_3[chi_te] == 'Chinstrap')  
## [1] 0.55  
  
mean(pred_3[gen_te] == 'Gentoo')  
## [1] 1
```

KNN ($k = 100$) Test Error

```
mean(pred_100[ade_te] == 'Adelie')  
## [1] 0.9387755  
  
mean(pred_100[chi_te] == 'Chinstrap')  
## [1] 0  
  
mean(pred_100[gen_te] == 'Gentoo')  
## [1] 1
```

Comparing Models: Think Goldilocks



Class	k=3	k=100	Logit
Adelie	0.75	0.93	0.83
Chinstrap	0.55	0.00	0.60
Gentoo	1.00	1.00	0.96

- ▶ Fit too closely to training data: $k = 3$
- ▶ Fit too loosely to training data: $k = 100$
- ▶ Fit just right to training data: logit (or maybe $3 < k < 100$)
- ▶ How can we formalize this goldilocks principle?

Bias Variance Tradeoff

Decomposing Error into Bias and Variance

Recall that the **bias** of an estimator is defined as follows:

$$\text{bias}(\hat{\theta}) \triangleq \mathbb{E} [\hat{\theta}] - \theta$$

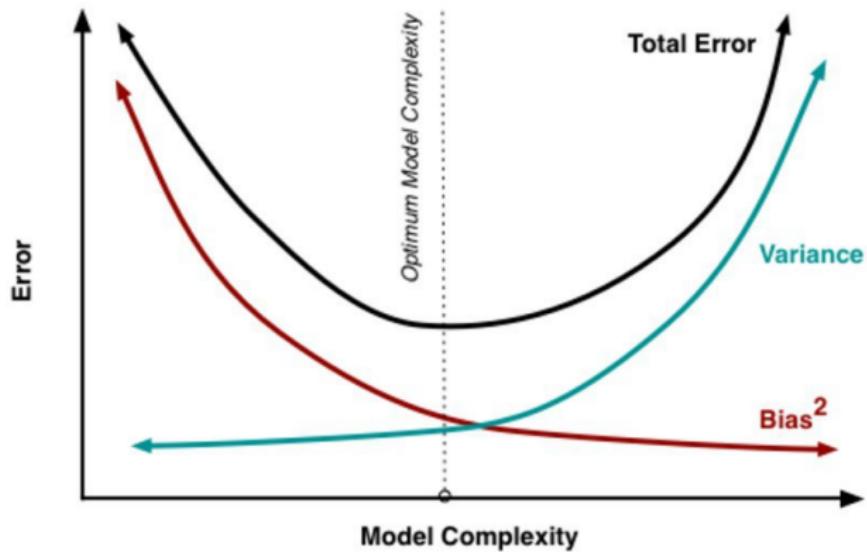
and the **variance** of an estimator is defined as follows:

$$\text{var}(\hat{\theta}) \triangleq \mathbb{E} [(\hat{\theta} - \mathbb{E} [\hat{\theta}])^2]$$

After some algebra (see the derivation here), we can decompose the expected error into bias squared and variance:

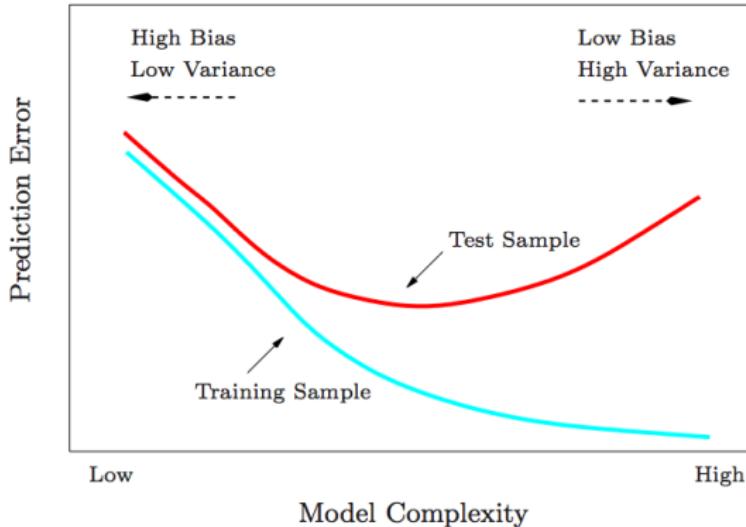
$$E [(f(x) - g(x))^2] = \text{bias}^2(g(x)) + \text{var}(g(x)) + \text{var}(\epsilon)$$

Model Complexity and the Bias-Variance Tradeoff



- ▶ As complexity of $g(x)$ increases, its **variance** increases and its **bias** decreases.
- ▶ Choosing the complexity based on average **test error** amounts to a **bias-variance trade-off**.

Model Complexity and the Bias-Variance Tradeoff



- ▶ Variance: the degree to which the functional form of $g(x)$ varies across datasets
- ▶ Bias: The inability of $g(x)$ to capture the true relationship due to modeling assumptions (e.g. linearity in linear regression).
- ▶ The goal is to find the sweet spot between a simple model and a complex model such that we balance bias and variance.

Intuition Behind Bias and Variance

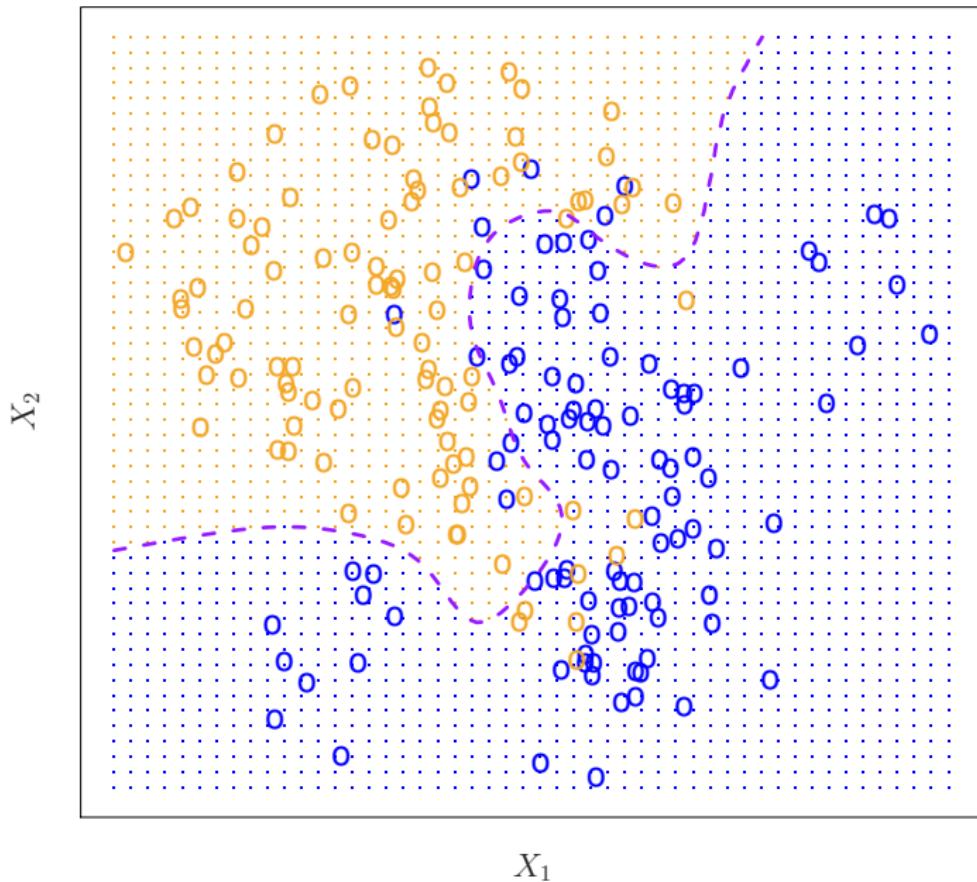
Models are biased when:

- ▶ Parametric: The form of the model does not incorporate all the necessary variables (omitted variable bias)
- ▶ Parametric: The functional form is too simple (e.g. a linear approximation)
- ▶ Non-parametric: The model provides too much smoothing.

Models are variable when:

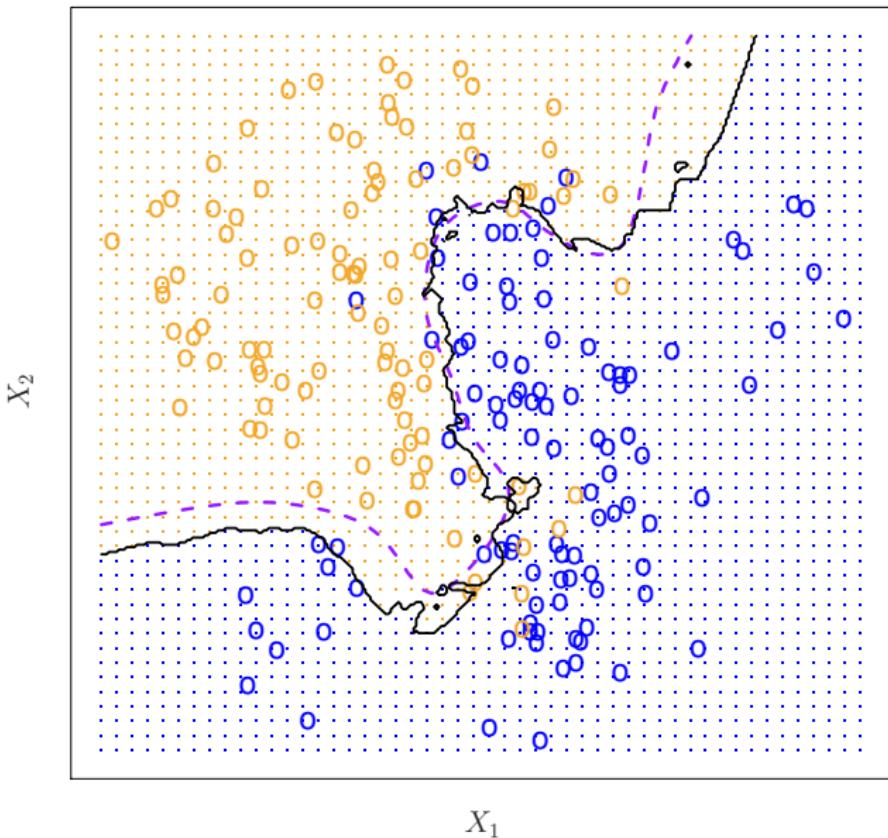
- ▶ Parametric: The form of the model incorporates too many variables.
- ▶ Parametric: The functional form is too complex.
- ▶ Non-parametric: The model does not provide enough smoothing.

Example: K-nearest neighbors in two dimensions



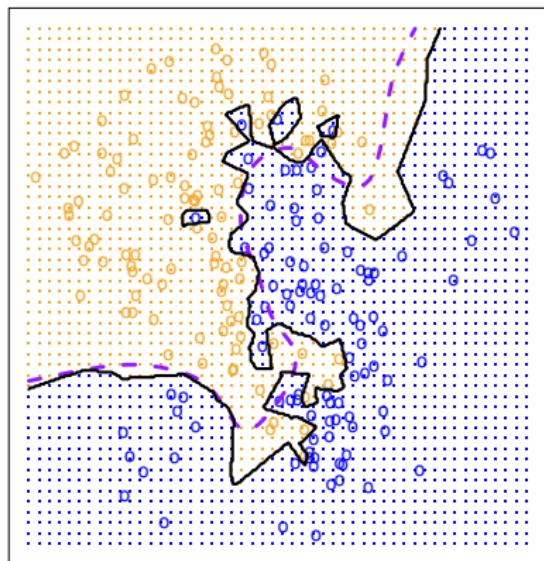
Example: K-nearest neighbors in two dimensions

KNN: K=10

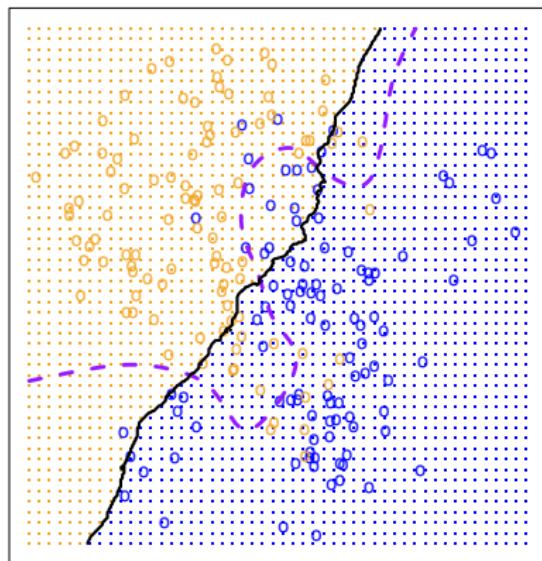


Example: K-nearest neighbors in two dimensions

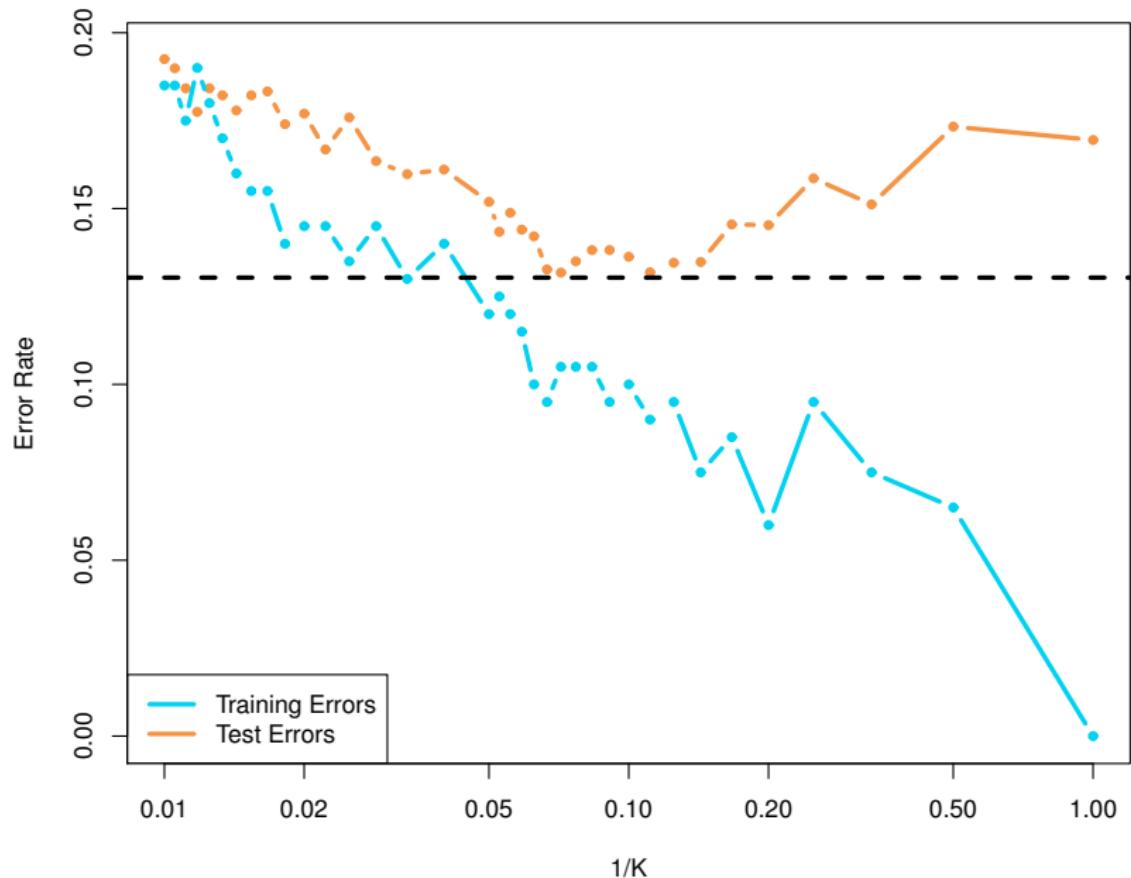
KNN: K=1



KNN: K=100



Example: K-nearest neighbors in two dimensions



Review: Modeling Non-Linear Relationships

- ▶ We can incorporate polynomial functions of the predictors to mitigate the effects of the linear assumption of a linear regression model.
- ▶ For example, in a scenario where a quadratic relationship seems likely, the following model could be used
- ▶ Read more about polynomial regression in ISL 3.3.2.

$$Y_i = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \epsilon$$

- ▶ This extension of the linear model to accommodate non-linear relationships is called **polynomial regression**.

Visualizing Bias and Variance

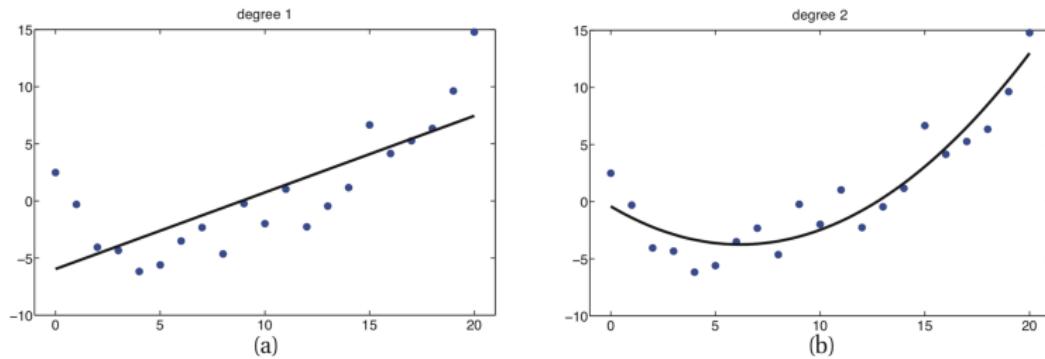


Figure 1.7 (a) Linear regression on some 1d data. (b) Same data with polynomial regression (degree 2). Figure generated by `linregPolyVsDegree`.

Source: *Machine Learning: A Probabilistic Perspective*

Visualizing Bias and Variance

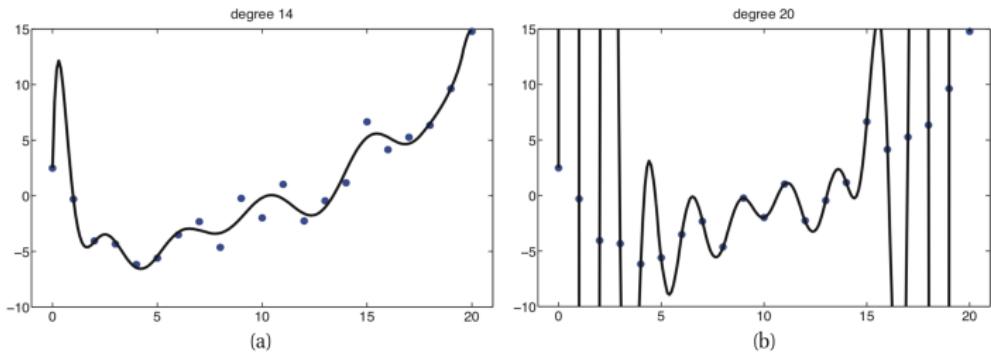
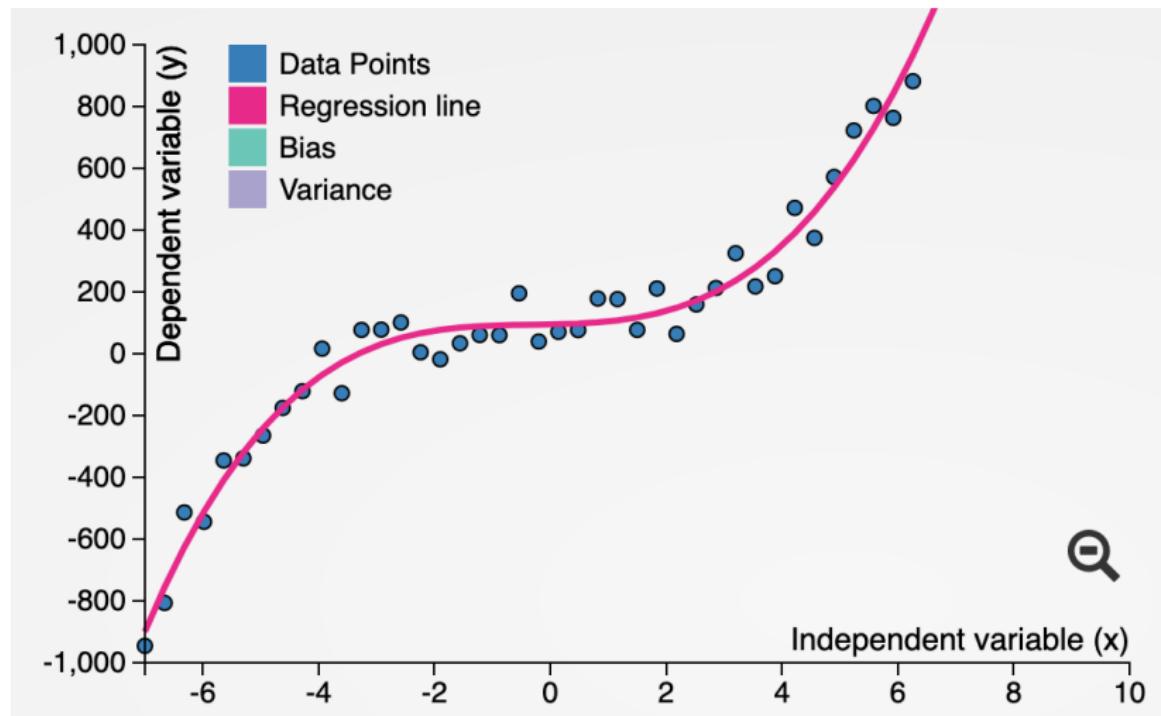


Figure 1.18 Polynomial of degrees 14 and 20 fit by least squares to 21 data points. Figure generated by `linregPolyVsDegree`.

Source: *Machine Learning: A Probabilistic Perspective*

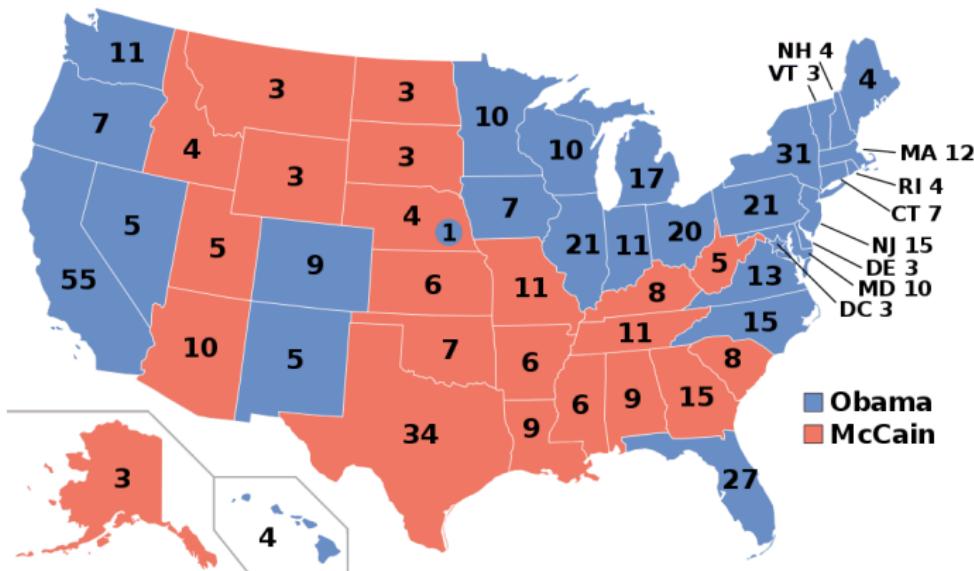
Visualizing Bias and Variance



Click here for the interactive demo.

Measuring Error

Motivating example: 2008 US Presidential Election



President Obama wins with 365 electoral votes to McCain's 173.

- ▶ In this example we will go over a prediction task that can be formulated as a **classification** and a **regression** problem
- ▶ The goal of this exercise is to make various **performance measures** or **measures of generalization error** clear.

Motivating example: 2008 US Presidential Election

- ▶ A number of pundits accurately predicted the 2008 election outcome.
- ▶ Electoral College system makes predicting election outcomes challenging.
 - ▶ Must win an absolute majority of electoral votes to be elected president
 - ▶ Each of the 538 electors casts a single electoral vote.
 - ▶ Most states have “winner-take-all” system.
 - ▶ A winning presidential candidate must obtain at least 270 electoral votes.
- ▶ **Goal:** predict election outcome using public opinion polls conducted within each state.
 - ▶ **The model:** Mean margin of all the polls on the latest day of polling in each state.

Election outcomes data (actual/y)

Variable	Description
state	abbreviated name of the state
state.name	unabbreviated name of the state
Obama	Obama's vote share (percentage)
McCain	McCain's vote share (percentage)
EV	number of Electoral College votes for the state
margin	Obama's margin

Election polling data (predicted/ \hat{y} /g(x))

Variable	Description
state	abbreviated name of the state
Obama	predicted support for Obama (percentage)
McCain	predicted support for McCain (percentage)
Pollster	name of the organization conducting the poll
middate	middate of the period when the poll was conducted
margin	Obama's margin
days	# days ahead of election the poll was conducted

Predicting vote margin from polls

Below we use the latest polls from each state to predict Obama's vote margin:

```
pres <- read.csv("pres08.csv")
polls <- read.csv("polls08.csv")

s_names <- unique(polls$state)
actual <- pres$margin
names(actual) <- as.character(s_names)
poll_pred <- rep(NA, 51)
names(poll_pred) <- as.character(s_names)

for (i in 1:51){
  s <- polls[polls$state == s_names[i], ]
  latest <- subset(s, days == min(days))
  poll_pred[i] <- mean(latest$margin)
}
```

Mean squared error of polls

```
head(poll_pred)
```

```
##      AL      AK      AZ      AR      CA      CO
## -25.0 -19.0  -2.5  -7.0  24.0   7.0
```

```
head(actual)
```

```
##  AL  AK  AZ  AR  CA  CO
## -21 -21  -9 -20  24   9
```

```
sq_err <- (poll_pred - actual)^2
```

```
head(sq_err)
```

```
##      AL      AK      AZ      AR      CA      CO
## 16.00  4.00 42.25 169.00  0.00  4.00
```

```
mean(sq_err)
```

```
## [1] 34.91558
```

Misclassification error rate of state predictions

```
pred <- ifelse(poll_pred > 0, "Obama", "McCain")
actual <- ifelse(pres$margin > 0, "Obama", "McCain")

mean(pred != actual)

## [1] 0.05882353

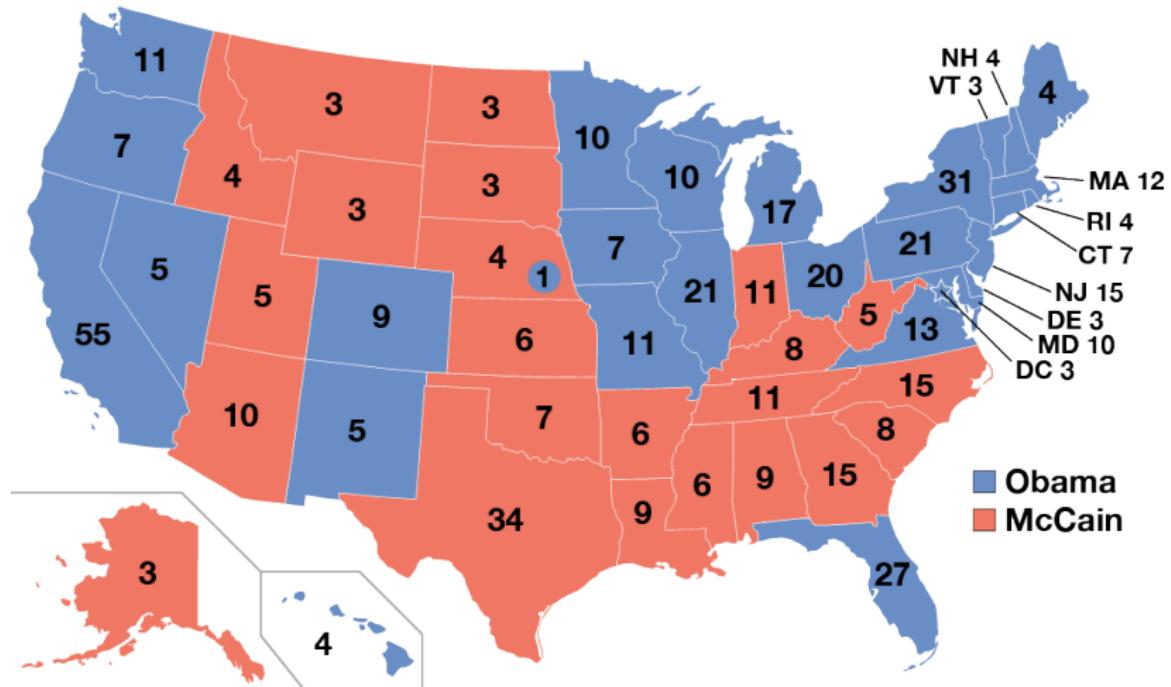
poll_pred[pred != actual]

## IN MO NC
## -5 1 -1

actual[pred != actual]

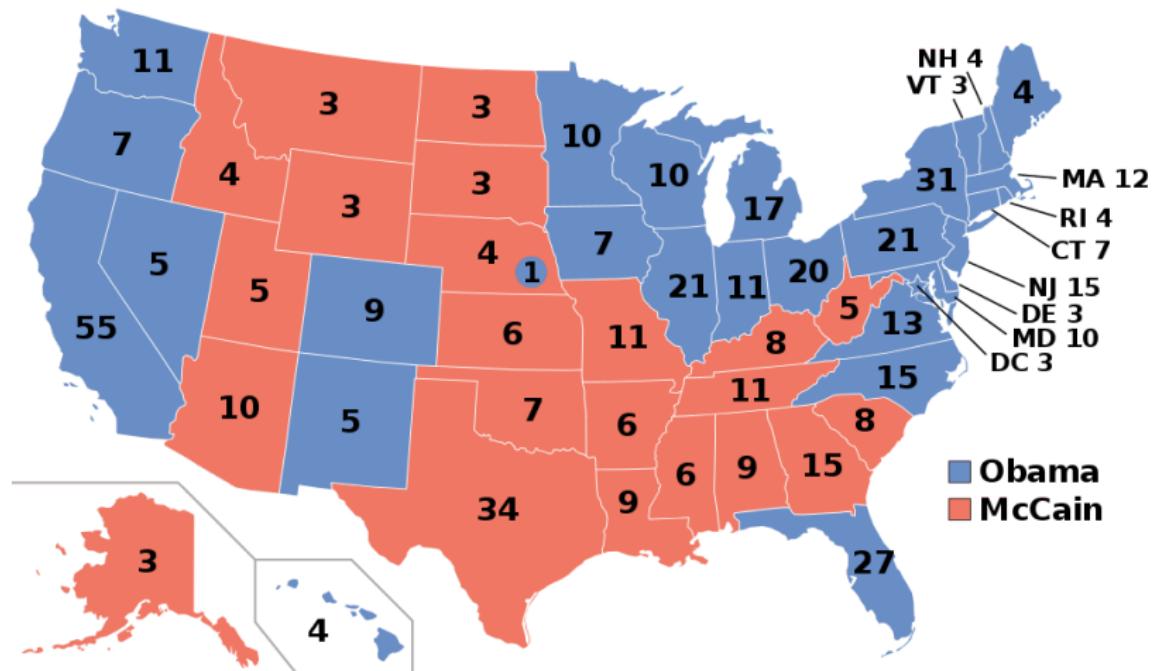
## [1] "Obama" "McCain" "Obama"
```

Our model's state predictions



President Obama wins with 349 electoral votes to McCain's 189.

Actual election outcome



President Obama wins with 365 electoral votes to McCain's 173.

Confusion matrix of state predictions

```
table(pred, actual)
```

```
##           actual
## pred      Obama McCain
##   Obama     27      1
##   McCain    2       21
```

- ▶ Rows correspond to what the model predicted, i.e. \hat{y}
- ▶ Columns correspond to the known truth, i.e. y

Confusion matrix of state predictions

```
table(pred, actual)
```

```
##           actual
## pred      Obama McCain
##   Obama     27      1
##   McCain    2      21
```

- ▶ Top left (**true positives**): predicted Obama states that were actually Obama states.
- ▶ Bottom right (**true negatives**): predicted McCain states that were actually McCain states.
- ▶ Top right (**false positives/Type I error**): predicted Obama states that were actually McCain states.
- ▶ Bottom left (**false negatives/Type II error**): predicted McCain states that were actually Obama states.

Class Balance and Error Measures

In the penguins example and the 2008 election example, the classes were more or less **balanced**.

```
table(penguins$species)
```

```
##  
##      Adelie Chinstrap     Gentoo  
##      146          68      119
```

```
table(actual)
```

```
## actual  
##   Obama McCain  
##      29      22
```

Class Balance and Error Measures

- ▶ COVID-19 tests are an example of an **imbalanced** classification problem.
- ▶ Data: emergency authorized rapid test reliability reported by the US Food and Drug Administration (FDA)
- ▶ In this problem $y \in \{\text{positive}, \text{negative}\}$. Thankfully, negative tests are much more common than positive tests:

```
covid <- read.csv('covid_tests.csv')  
mean(covid$tp + covid$fn)
```

```
## [1] 33.57447
```

```
mean(covid$tn + covid$fp)
```

```
## [1] 82.10638
```

- ▶ In this case, accuracy is probably not a great metric of test reliability

Class Balance and Error Measures

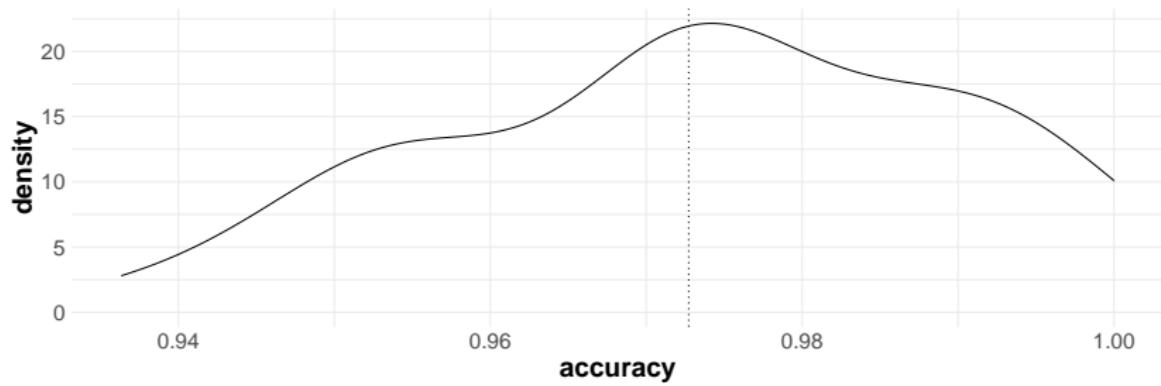
```
total <- (covid$tn + covid$tp + covid$fn + covid$fp)
covid$accuracy <- (covid$tn + covid$tp) / total
median(covid$accuracy)
```

```
## [1] 0.9727273
```

```
mean(covid$accuracy)
```

```
## [1] 0.973863
```

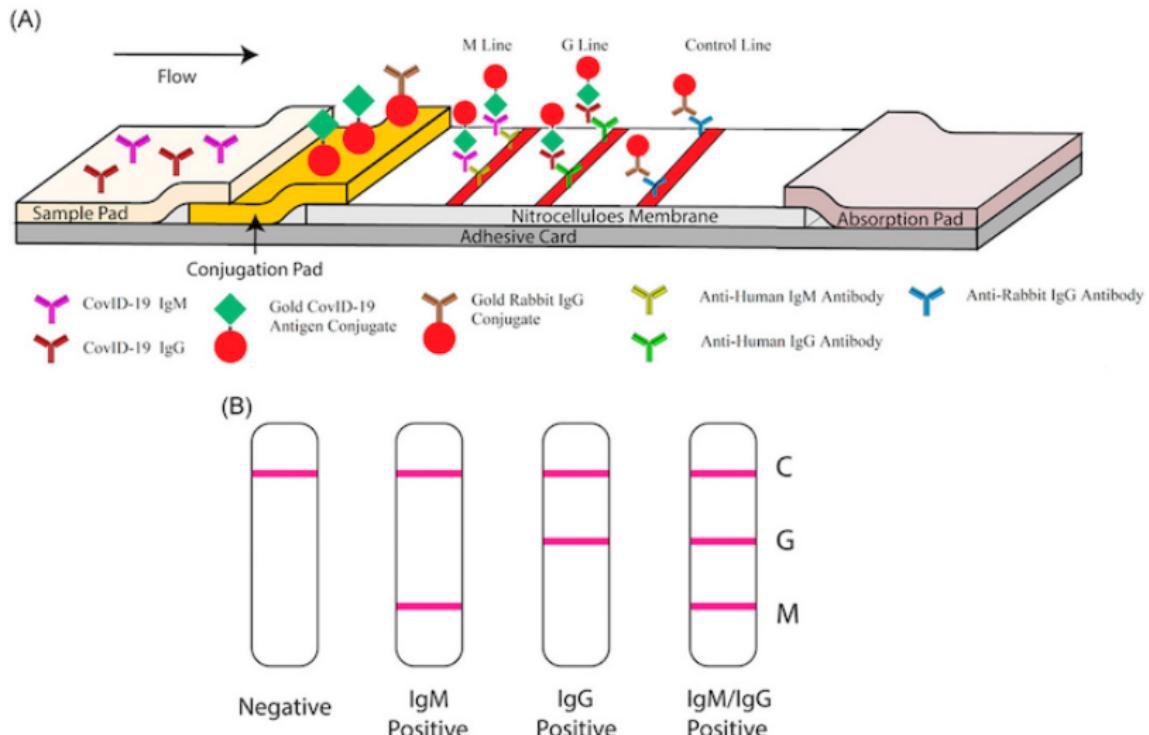
Density Plot of Test Accuracy



A Thought Experiment

- ▶ Between 28 May and 7 October, NHS Test and Trace reports that 6.3% of people tested had a positive result.
- ▶ Imagine we are fraudsters, and develop a ridiculously cheap (but useless) test for COVID-19 antibodies that always returns “negative.” We would have an accuracy of 92.7%.
- ▶ While this is below the accuracy of the FDA-approved rapid antibody tests, we might be able to fool some people with an accuracy in the 90s!
- ▶ This is why accuracy is not used to assess the reliability of medical tests.
- ▶ Instead, **sensitivity** and **specificity** are the standard metrics:
 - ▶ Sensitivity: Rate at which the test was positive for those who have COVID-19 antibodies.
 - ▶ Specificity: Rate at which the test was negative for those who do not have COVID-19 antibodies.

Lateral Flow COVID-19 Antibody Test



Source: Nguyen, Ngan NT, et al. "Development of Diagnostic Tests for Detection of SARS-CoV-2." *Diagnostics* 10.11 (2020): 905.

Lateral Flow COVID-19 Antibody Test



- ▶ Swab of nose and/or mouth is mixed with a buffer solution
- ▶ Some of the solution is dropped on the lateral flow device
- ▶ The solution flows across an absorbent strip via capillary action
- ▶ The strip contains two or more lines depending on how many antibody targets there are
 - ▶ One control line to demonstrate that the test has worked as expected
 - ▶ One or more test line containing lab-created antibodies that will bind to specific COVID-19 antibodies

AbC-19 Rapid Test



Antibody tests bought by UK government 'less accurate than maker claims'

Abingdon Health claimed test was 99% accurate but PHE puts its real-world accuracy at 84.7%

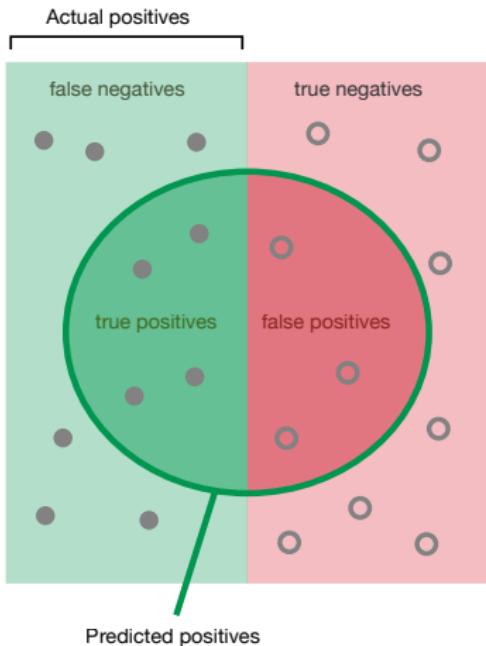
Source: [The Guardian](#)

- ▶ UK Government placed an order for one million AbC-19 tests
- ▶ The manufacturer claimed specificity of 100% but [later independent studies](#) suggest the correct number is 84.7%
- ▶ This means there is a false positive rate of 15.3%

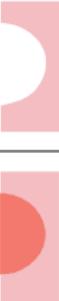
Confusion matrix

		Actual Positive	Actual Negative
Predicted Positive	True Positive	False Positive	Precision = $\frac{TP}{TP + FP}$
	False Negative	True Negative	
Predicted Negative			Recall = $\frac{TP}{TP + FN}$

Performance measures: Specificity



How often are actual negatives predicted to be negative?

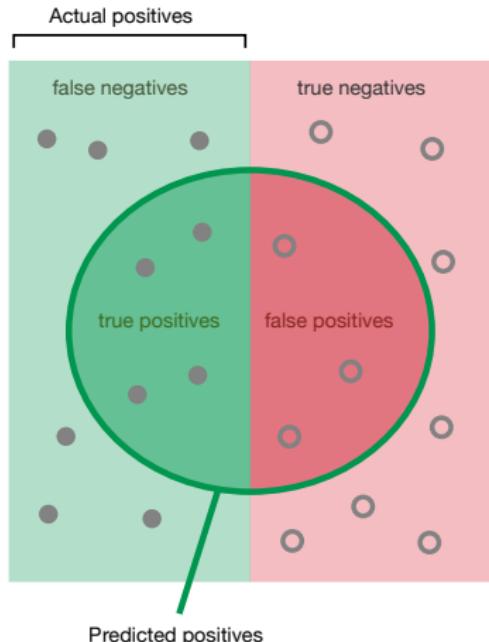
$$\text{Specificity} = \frac{\text{true negatives}}{\text{true negatives} + \text{false positives}} = \frac{7}{10} = .7$$


Performance measures: Specificity

```
covid$sp <- with(covid, tn/(tn + fp))
p <- ggplot(covid, aes(x=sp, fill=ab))
p <- p + geom_histogram(alpha=0.25, bins=5) + theme
p + geom_vline(xintercept=median(covid$sp))
```



Performance measures: Recall/Sensitivity/True Positive Rate



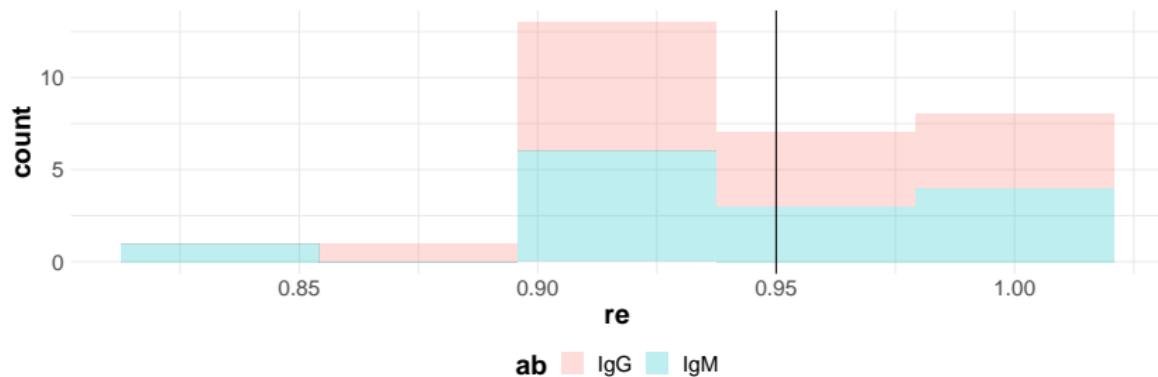
What proportion of the actual positives are predicted to be positive?

$$\text{Recall} = \frac{\text{true positives}}{\text{actual positives}} = \frac{4}{10} = .4$$

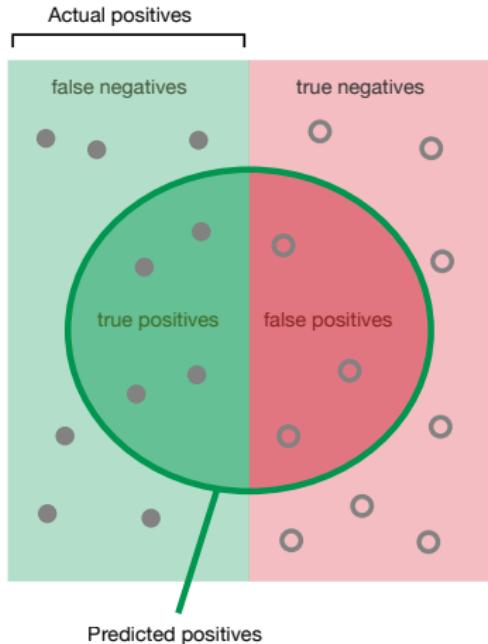
Recall = $\frac{\text{true positives}}{\text{actual positives}} = \frac{4}{10} = .4$

Performance measures: Recall/Sensitivity/True Positive Rate

```
covid$re <- with(covid, tp/(tp + fn))
p <- ggplot(covid, aes(x=re, fill=ab))
p <- p + geom_histogram(alpha=0.25, bins=5) + theme
p + geom_vline(xintercept=median(covid$re))
```



Performance measures: Precision



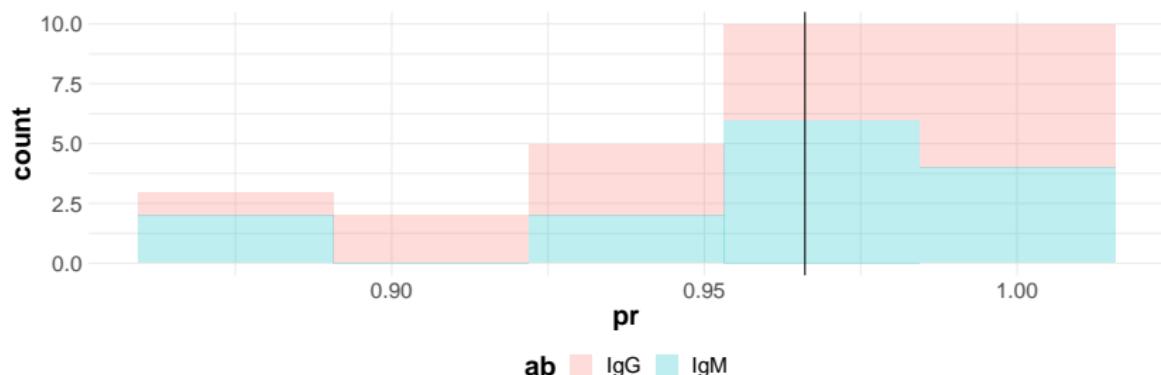
What proportion of predicted positives are in fact positive?

$$\text{Precision} = \frac{\text{true positives}}{\text{predicted positives}} = \frac{4}{7} = .57$$

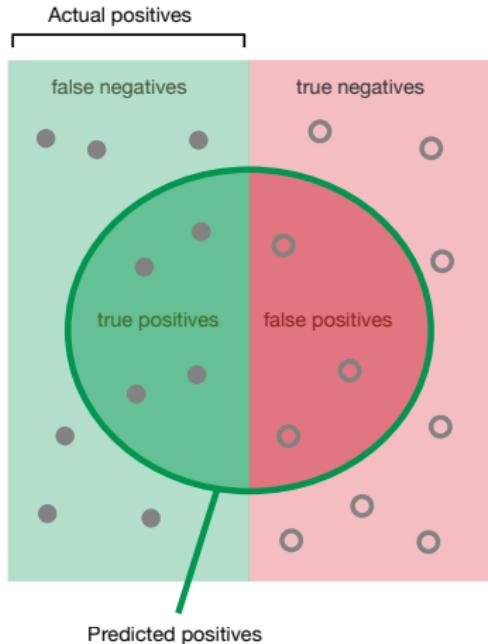
A pie chart illustrating the proportion of predicted positives that are true positives. The chart is divided into two equal halves: green and red. This visualizes the fraction 4/7, which corresponds to the precision value of .57.

Performance measures: Precision

```
covid$pr <- with(covid, tp/(tp + fp))
p <- ggplot(covid, aes(x=pr, fill=ab))
p <- p + geom_histogram(alpha=0.25, bins=5) + theme
p + geom_vline(xintercept=median(covid$pr))
```



Performance measures: False Positive Rate



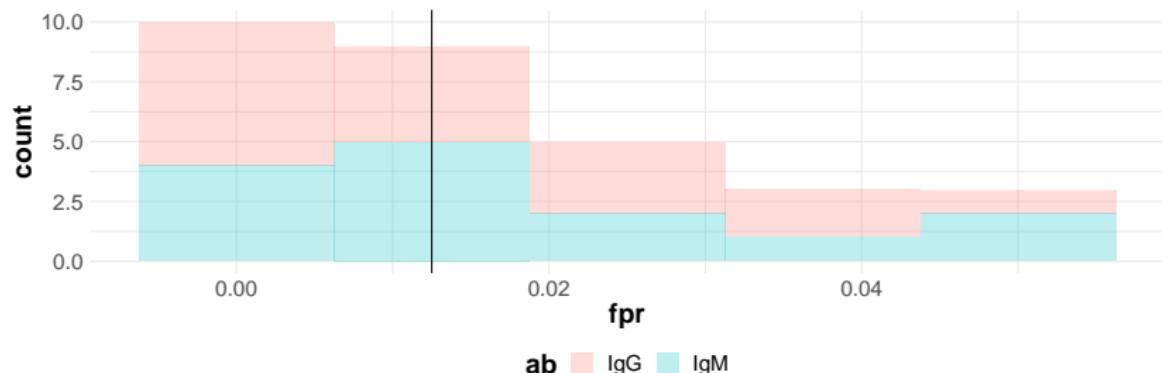
What proportion of actual negatives are predicted to be positive?

$$\text{False Positive Rate} = \frac{\text{false positives}}{\text{actual negatives}} = 3/10 = .3$$



Performance measures: False Positive Rate

```
covid$fpr <- with(covid, fp/(tn + fp))
p <- ggplot(covid, aes(x=fpr, fill=ab))
p <- p + geom_histogram(alpha=0.25, bins=5) + theme
p + geom_vline(xintercept=median(covid$fpr))
```



Performance measures: F_1 , F_k

- ▶ F_1 is a performance measure that balances **precision** and **recall**:

$$F_1 = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

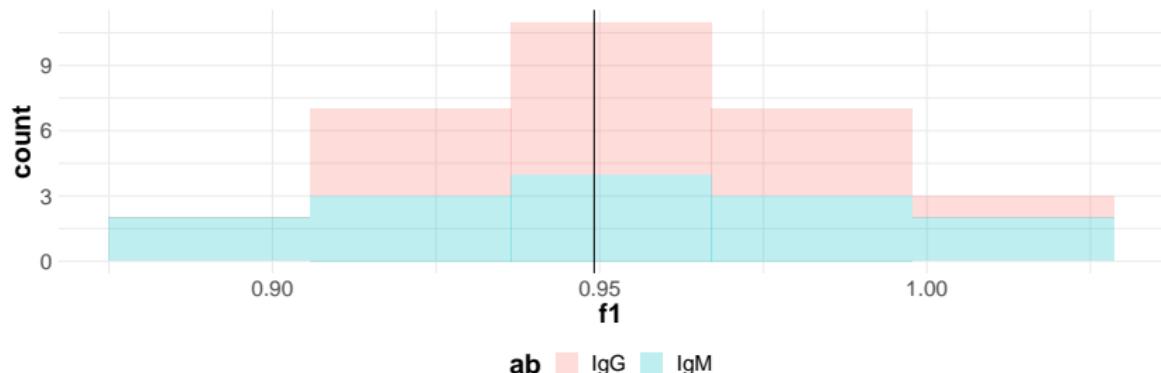
- ▶ F_1 is the **harmonic mean** of the two measures.
- ▶ The “1” in F_1 represents a parameter that can be adjusted to weight the relative importance of precision and recall:

$$F_k = (1 + k^2) \cdot \frac{\text{precision} \cdot \text{recall}}{k^2 \cdot \text{precision} + \text{recall}}$$

- ▶ A bigger k weights recall higher than precision; a smaller k weights precision higher than recall.

Performance measures: F_1

```
covid$f1 <- with(covid, 2 * (pr * re)/(pr + re))
p <- ggplot(covid, aes(x=f1, fill=ab))
p <- p + geom_histogram(alpha=0.25, bins=5) + theme
p + geom_vline(xintercept=median(covid$f1))
```



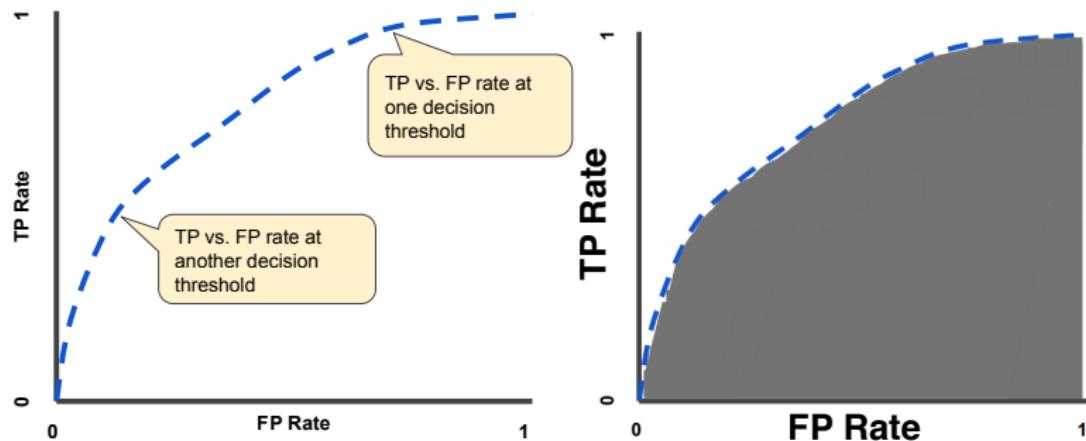
Area under the receiver operator curve (AUC)



Sailors operating a 285 gunnery radar. Photo by William H. Pugsley. National Archives of Canada, PA-139273.

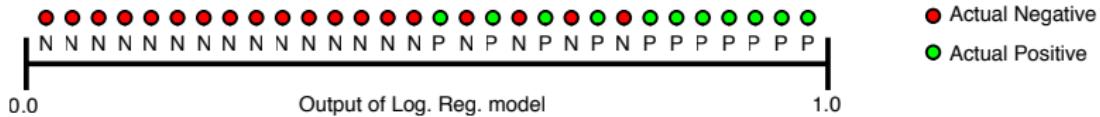
- ▶ ROC was first used in World War II to aid in the detection of enemy submarines
- ▶ A true positive (enemy submarine) needed to be distinguished from a false positive (whales, fish, etc.)

Area under the receiver operator curve (AUC)



- ▶ Left: True positive rate vs. false positive rate at different classification thresholds.
- ▶ Right: Area under the ROC Curve.
- ▶ The curve is then defined by the false positive rate and false negative rate if that predicted outcome were to represent the **classification threshold**.

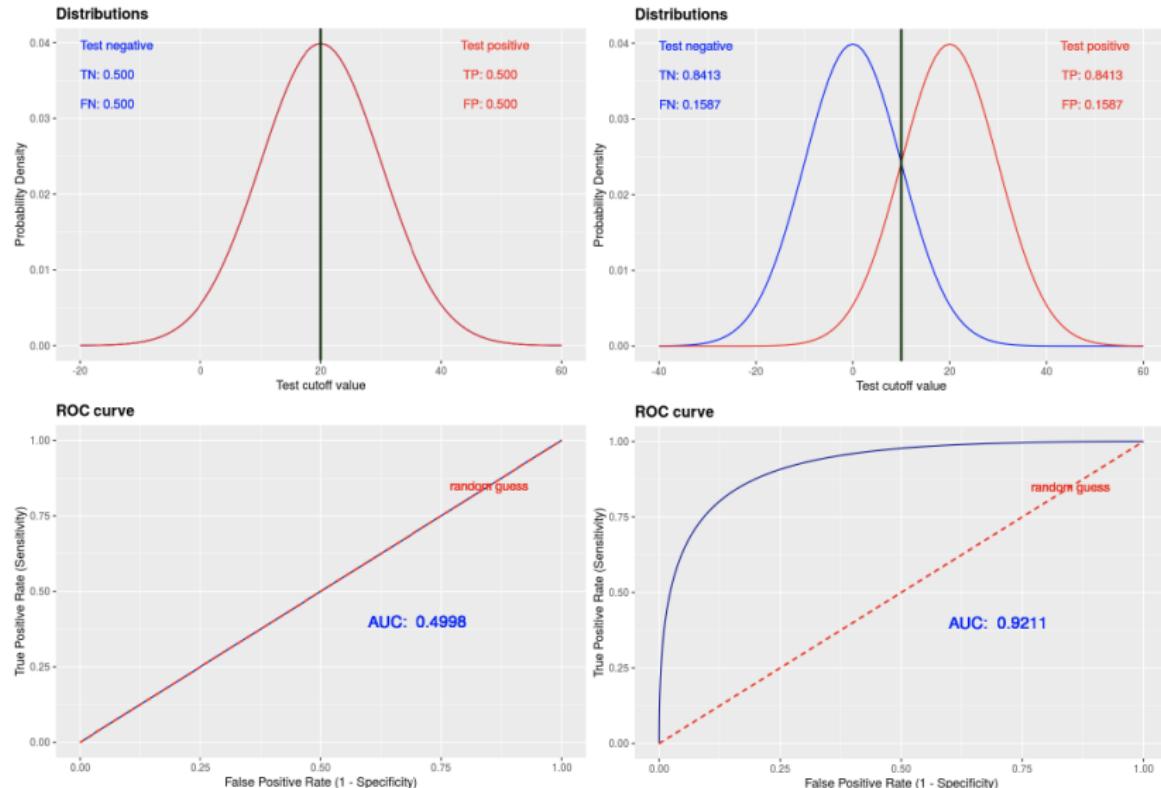
Area under the receiver operator curve (AUC)



Predictions from a logistic regression model ordered by predicted probability. Source: developers.google.com

- ▶ ROC curve ranks all observations in the order of their predicted outcome (for example predicted probabilities of a logistic regression model).
 - ▶ AUC can be interpreted as the probability that a randomly drawn positive (green) observation is positioned to the right of a randomly drawn negative (red) observation.

Area under the receiver operator curve (AUC)



[Click here for an interactive demo.](#)

Quiz Review

Review Questions: Error Measures

1. Think of a classification problem where accuracy is a bad error measure.
2. Why do we need both sensitivity AND specificity?
 - ▶ How could one commit fraud by only reporting one of these values when selling an unreliable COVID test?

Review Questions: “Big Data”

1. How might “big data” aid in social science research?
2. What are the limitations of big data approaches?
3. What must we be cautious about when using “big data?”

Review Questions: Causal Inference

1. Why might one argue that “big p ” data could solve the fundamental problem of causal inference?
2. Why might one argue that “big n ” data could solve the fundamental problem of causal inference?

Takeaways

1. Big data cannot make up for poor theory and research design
2. Big data facilitate rich description, exploration, and hypothesis generation
3. Big data can accelerate of the process of hypothesis generation.
4. “As more phenomena become quantifiable, the range of implications of scientific theories that can be tested empirically is expanded significantly.”