
Jake's pups!

Lalita's photography!

Logistic regression

Data Science for Biologists

Dr. Spielman

Make it fit better on slides

```
penguins %>%
  rename(bill_len = bill_length_mm,
         bill_dep = bill_depth_mm,
         flipper = flipper_length_mm,
         mass    = body_mass_g) -> peng

peng
```

```
## # A tibble: 344 x 8
##    species island    bill_len bill_dep flipper  mass sex     year
##    <fct>   <fct>        <dbl>    <dbl>   <int> <int> <fct>  <int>
##  1 Adelie  Torgersen     39.1     18.7     181  3750 male    2007
##  2 Adelie  Torgersen     39.5     17.4     186  3800 female  2007
##  3 Adelie  Torgersen     40.3     18       195  3250 female  2007
##  4 Adelie  Torgersen     NA       NA        NA    NA <NA>    2007
##  5 Adelie  Torgersen     36.7     19.3     193  3450 female  2007
##  6 Adelie  Torgersen     39.3     20.6     190  3650 male    2007
##  7 Adelie  Torgersen     38.9     17.8     181  3625 female  2007
##  8 Adelie  Torgersen     39.2     19.6     195  4675 male    2007
##  9 Adelie  Torgersen     34.1     18.1     193  3475 <NA>    2007
## 10 Adelie  Torgersen     42       20.2     190  4250 <NA>    2007
## # … with 334 more rows
```

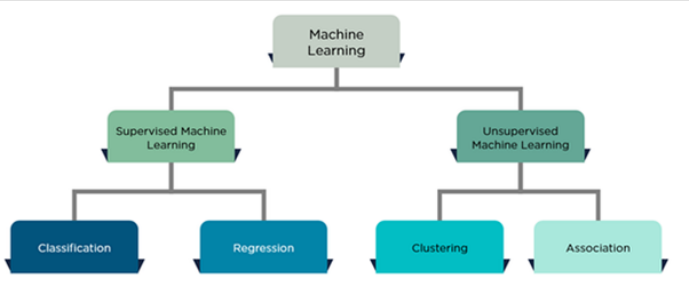
Linear regression vs. logistic regression

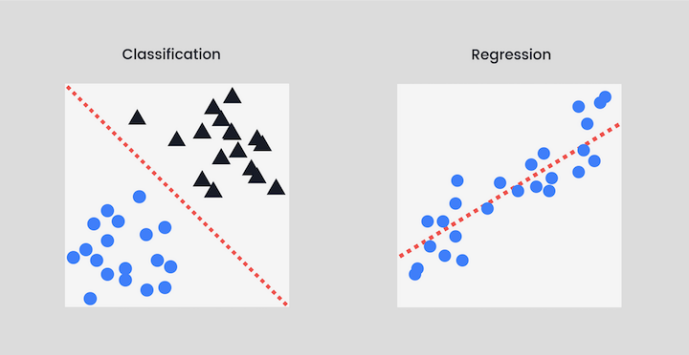
- Linear regression: How much do these (linearly-related) predictors explain variation in my *numeric* response variable?

- Logistic regression: How well do these predictors explain variation in my *categorical* ***binary*** response variable?
  - E.g. predicting Species in the iris dataset would be a categorical predictor, but NOT binary
  - Type of classifier

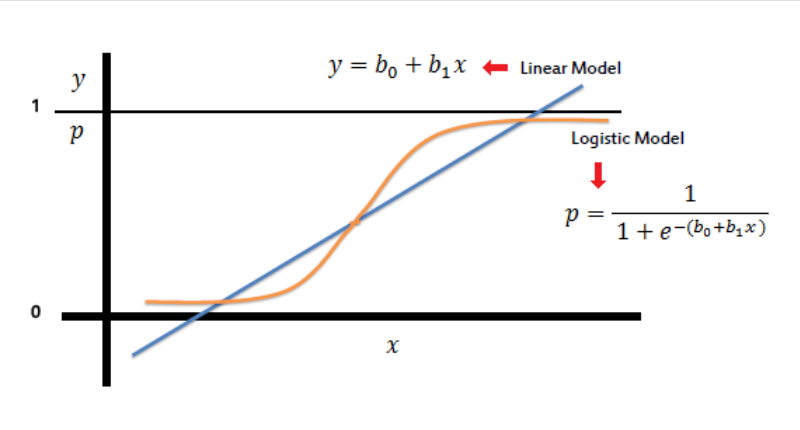
Where are we in the "machine learning" universe?

- Machine learning = the computer learns through experience
  - More data = more experience! *Training models on data IS machine learning*
  - Ignore the AI hype.





Logistic regression



- Linear regression: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 \ldots + \beta_N X_N + \epsilon$
- Logistic regression *transforms the predictors*
  - $t = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 \ldots + \beta_N X_N + \epsilon$
  - $Y = \frac{1}{1+e^{-t}}$ (or, $p = \ldots$ in image)

```r
library(palmerpenguins) # to access penguins dataset

## Make it fit better on slides
penguins%>%
  rename(bill_len = bill_length_mm,
         bill_dep = bill_depth_mm,
         flipper = flipper_length_mm,
         mass    = body_mass_g) %>%
  # appease the step() function gods
  drop_na()-> peng_nona

peng_nona
```

```
## # A tibble: 333 x 8
##    species island    bill_len bill_dep flipper  mass sex     year
##    <fct>   <fct>        <dbl>    <dbl>   <int> <int> <fct>  <int>
##  1 Adelie  Torgersen     39.1     18.7     181  3750 male    2007
##  2 Adelie  Torgersen     39.5     17.4     186  3800 female  2007
##  3 Adelie  Torgersen     40.3     18       195  3250 female  2007
##  4 Adelie  Torgersen     36.7     19.3     193  3450 female  2007
##  5 Adelie  Torgersen     39.3     20.6     190  3650 male    2007
##  6 Adelie  Torgersen     38.9     17.8     181  3625 female  2007
##  7 Adelie  Torgersen     39.2     19.6     195  4675 male    2007
##  8 Adelie  Torgersen     41.1     17.6     182  3200 female  2007
##  9 Adelie  Torgersen     38.6     21.2     191  3800 male    2007
## 10 Adelie  Torgersen     34.6     21.1     198  4400 male    2007
## # … with 323 more rows
```

Goal: Can we predict a penguin's sex?

```
## Sex is a binary variable in the penguins data:
levels(peng_nona$sex)
```

```
## [1] "female" "male"
```

Step 1: Prepare the data

```
## To appease the R gods, and make your life easier, ...
## re-code the response as arbitrary success = 1, failure = 0.
peng_nona %>%
  # change `sex` to be 0, 1
  mutate(sex = if_else(sex == "female", 1, 0)) -> peng_nona_sex01

peng_nona_sex01
```

```
## # A tibble: 333 x 8
##    species island    bill_len bill_dep flipper  mass   sex  year
##    <fct>   <fct>        <dbl>    <dbl>   <int> <int> <dbl> <int>
##  1 Adelie  Torgersen     39.1     18.7     181  3750     0  2007
##  2 Adelie  Torgersen     39.5     17.4     186  3800     1  2007
##  3 Adelie  Torgersen     40.3     18       195  3250     1  2007
##  4 Adelie  Torgersen     36.7     19.3     193  3450     1  2007
##  5 Adelie  Torgersen     39.3     20.6     190  3650     0  2007
```

Step 2: Build the model

`glm(response ~ predictors, data = data, family = "binomial")`

- Use function `glm()`
- Include argument `family = "binomial"`
- Everything else is the same!

```
## Use model selection to identify optimal predictors
initial_fit <- glm(sex ~ ., data = peng_nona_sex01, family = "binomial")
fit <- step(initial_fit, trace = FALSE)
```

Interpreting the logistic regression coefficients

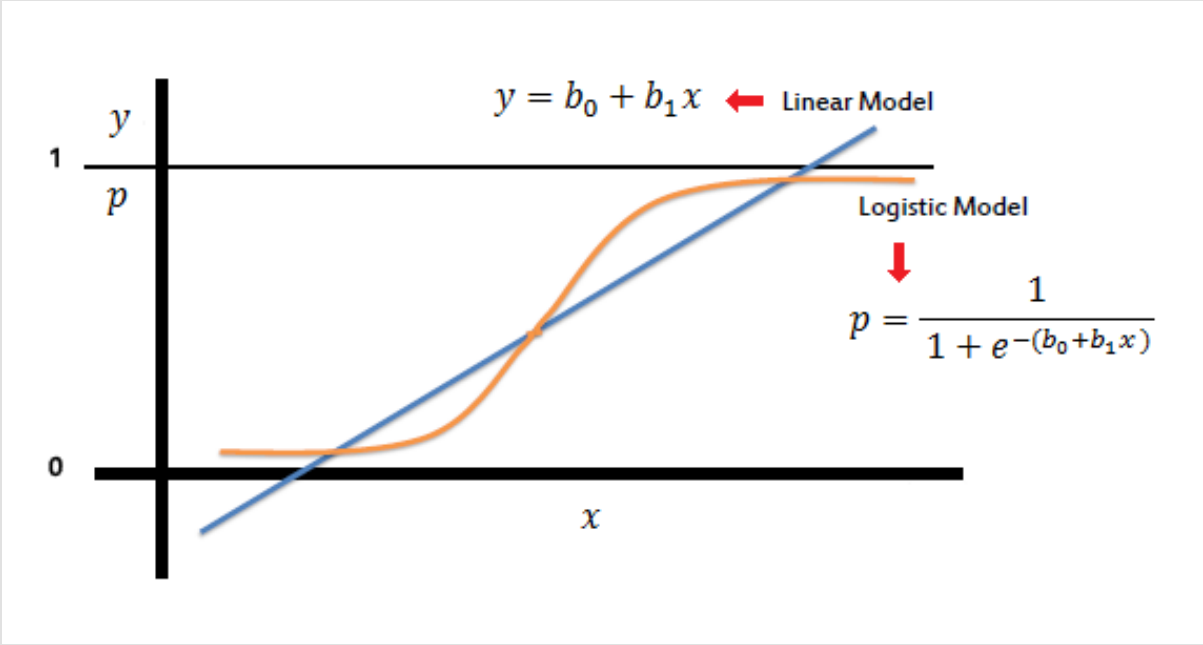
> Protip: Don't.

```
tidy(fit)
```

```
## # A tibble: 6 x 5
##   term             estimate std.error statistic  p.value
##   <chr>               <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)      76.1       9.80         7.76 8.34e-15
## 2 speciesChinstrap  6.90      1.56         4.43 9.56e- 6
## 3 speciesGentoo     7.88      2.25         3.50 4.62e- 4
## 4 bill_len         -0.620     0.131       -4.74 2.11e- 6
## 5 bill_dep         -1.64      0.331       -4.97 6.69e- 7
## 6 mass             -0.00596   0.00106     -5.62 1.88e- 8
```

- For every unit increase in the predictor, the **log odds of success** of the response increases by the coefficient
  - $Pr(success)$ = probability of being *female* for a given set of observations (predictors)
  - $Pr(failure)$ = probability of being *male* for a given set of observations
  - **Log odds** = $ln\left(\frac{Pr(success)}{Pr(failure)}\right)$

Visualizing the fitted logistic curve ("the model")



```
## USING head() to make it fit on slides!!

## YOUR X-AXIS !!
## What would have been your Y-values if this were regression
head(fit$linear.predictors)
```

```
##          1          2          3          4          5          6
## -1.2431192  0.3474612  2.1441466  1.0474121 -3.8938334  1.1053579
```

```
## YOUR Y-AXIS !!
## The logit transformed - PROBABILITIES OF SUCCESS
head(fit$fitted.values)
```

```
##          1          2          3          4          5          6
## 0.22389350 0.58600180 0.89512053 0.74027765 0.01996058 0.75126267
```

- $t = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 \ldots + \beta_N X_N + \epsilon$
- $Y = \frac{1}{1+e^{-t}}$

```
1/(1 + exp(-1 * fit$linear.predictors)) %>% head()
```

```
##          1          2          3          4          5          6
## 0.22389350 0.58600180 0.89512053 0.74027765 0.01996058 0.75126267
```

Visualizing the model: Prepare the data

```
tibble(x = fit$linear.predictors,
       y = fit$fitted.values,
       sex = peng_nona$sex) -> fit_tibble

fit_tibble
```

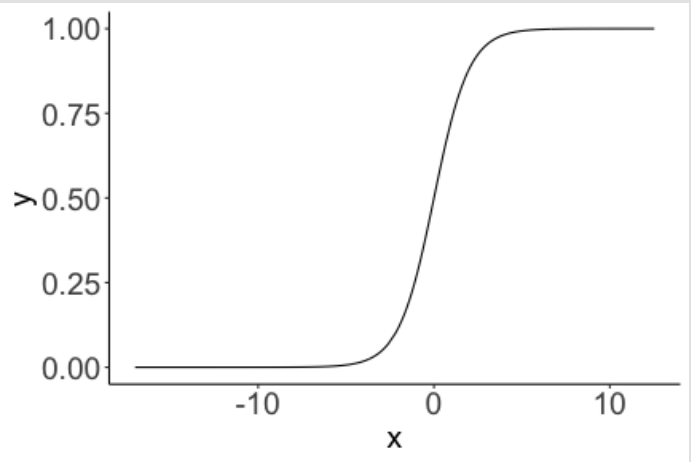
```
## # A tibble: 333 x 3
##         x        y sex
##     <dbl>    <dbl> <fct>
##  1 -1.24  0.224    male
##  2  0.347 0.586    female
##  3  2.14  0.895    female
##  4  1.05  0.740    female
##  5 -3.89  0.0200   male
##  6  1.11  0.751    female
##  7 -8.30  0.000249 male
##  8  2.60  0.931    female
##  9 -5.34  0.00477  male
## 10 -6.27  0.00188  male
## # … with 323 more rows
```

Visualizing the model

```
head(fit_tibble)
```

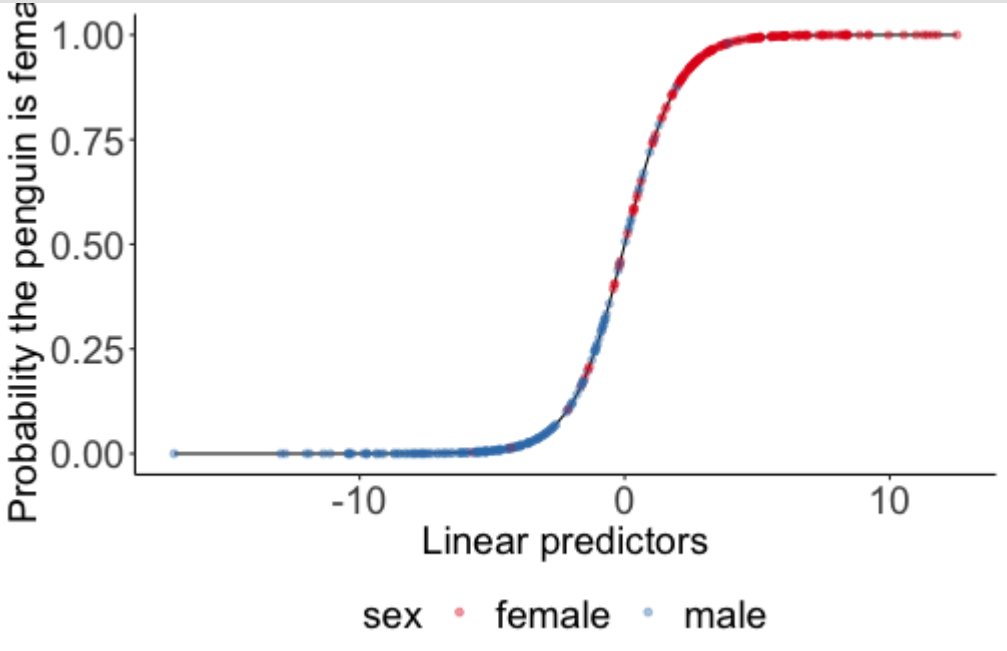
```
## # A tibble: 6 x 3
##        x      y sex
##    <dbl>  <dbl> <fct>
## 1 -1.24  0.224  male
## 2  0.347 0.586  female
## 3  2.14  0.895  female
## 4  1.05  0.740  female
## 5 -3.89  0.0200 male
## 6  1.11  0.751  female
```

```
ggplot(fit_tibble, aes(x = x, y = y)
 geom_line()
```



Visualizing the model *fully*

```
ggplot(fit_tibble, aes(x = x, y = y)) +
 geom_line() +
geom_point(aes(color = sex), alpha = 0.4) +
 scale_color_brewer(palette = "Set1") +
 theme(legend.position = "bottom") +
  labs(x = "Linear predictors",
       y = "Probability the penguin is female")
```



Confusion matrix time

	Predicted 0	Predicted 1
Actual 0	TN	FP
Actual 1	FN	TP

- **First ask:** is the result positive or negative?
  - "Successes" are positive and "failures" are negative.
- **Then ask:** should we have gotten that result though?
  - If yes, *TRUE*. If not, *FALSE*.

What is it?

A new arthritis drug does help pain clinical trials, even though it actually does reduce arthritis pain.

A person with HIV receives a positive test result for HIV.

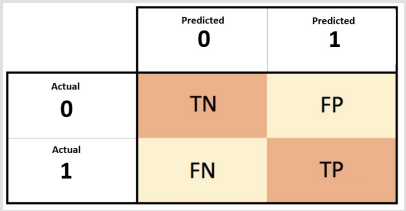
A person using illegal performing enhancing drugs passes a test clearing them of drug use.

A study found a significant relationship between neck strain and jogging, when reality there is no relationship.

A healthy individual gets a positive cancer biopsy result.

Classification metrics (an abbreviated set)

- True positive rate:



$TPR = TP/P = \frac{TP}{TP+FN}$

  - AKA *sensitivity* AKA *recall*
- True negative rate: $TNR = TN/N = \frac{TN}{FP+TN}$
  - AKA *specificity*
- False positive rate: $FPR = FP/N = \frac{FP}{FP+TN}$
  - AKA *1 - specificity*

- Precision: $PPV = \frac{TP}{TP+FP}$
  - AKA *positive predictive value*
- Accuracy: $\frac{TP+TN}{TP+TN+FP+FN}$

Recall our model:

```
## Recall:
peng_nona %>%
  mutate(sex = if_else(sex == "female", 1, 0)) -> peng_nona_sex01
initial_fit <- glm(sex ~ ., data = peng_nona_sex01, family = "binomial")
fit <- step(initial_fit, trace = FALSE)

tibble(x = fit$linear.predictors,
       y = fit$fitted.values,
       sex = peng_nona$sex) -> fit_tibble

head(fit_tibble)
```

```
## # A tibble: 6 x 3
##        x      y sex
##    <dbl>  <dbl> <fct>
## 1 -1.24  0.224  male
## 2  0.347 0.586  female
## 3  2.14  0.895  female
## 4  1.05  0.740  female
## 5 -3.89  0.0200 male
## 6  1.11  0.751  female
```

Caculating performance measures

- Requires a *threshold* to call female/male model outcomes.
- For an example, let's say >=0.75 is female (arbitrary "success"). <0.75 is male (arbitrary "failure")
- Accuracy: $\frac{TP+TN}{TP+TN+FP+FN}$

```
threshold <- 0.75
fit_tibble %>%
  rename(truth = sex) %>%
  mutate(pred = if_else(y >= threshold, "female", "male"))
```

```
## # A tibble: 333 x 4
##         x        y truth  pred
##     <dbl>    <dbl> <fct>  <chr>
##  1 -1.24  0.224    male   male
##  2  0.347 0.586    female male
##  3  2.14  0.895    female female
##  4  1.05  0.740    female male
##  5 -3.89  0.0200   male   male
##  6  1.11  0.751    female female
##  7 -8.30  0.000249 male   male
##  8  2.60  0.931    female female
##  9 -5.34  0.00477  male   male
## 10 -6.27  0.00188  male   male
## # … with 323 more rows
```

Detour: let's learn about `case_when()`

What if we want to do `if_else()` but with more than two options?

```
tibble(grades =
         c(95, 88, 83, 91, 79, 72, 8
```

```
## # A tibble: 7 x 1
##   grades
##    <dbl>
## 1     95
## 2     88
## 3     83
## 4     91
## 5     79
## 6     72
## 7     87
```

- `>90` is "A"
- `>=80 & < 90` is "B"
- `>=70 & < 80` is "C"
- `>=60 & < 70` is "D"
- Rest is "F"

- `>90` is "A"
- `>=80 & < 90` is "B"
- `>=70 & < 80` is "C"
- `>=60 & < 70` is "D"
- Rest is "F"

```
tibble(grades = c(95, 88, 83, 91, 79, 72, 87)) %>%
  mutate(letter_grade = case_when(grades > 90 ~ "A",
                                  grades >=80 & grades < 90 ~ "B",
                                  grades >=70 & grades < 80 ~ "C",
                                  grades >=60 & grades < 70 ~ "D",
                                  TRUE ~ "F")
         ) # close mutate() parentheses
```

```
## # A tibble: 7 x 2
##   grades letter_grade
##    <dbl> <chr>
## 1     95 A
## 2     88 B
## 3     83 B
## 4     91 A
## 5     79 C
## 6     72 C
## 7     87 B
```

```r
threshold <- 0.75
fit_tibble %>%
  rename(truth = sex) %>%
  mutate(pred = if_else(y >= threshold, "female", "male")) %>%
  # female is positive, male is negative
  mutate(classif = case_when(truth == "female" & pred == "female" ~ "TP",
                             truth == "female" & pred == "male" ~ "FN",
                             truth == "male"    & pred == "female" ~ "FP",
                             truth == "male"    & pred == "male" ~ "TN")) ->

confusion
```

```
## # A tibble: 333 x 5
##         x        y truth  pred   classif
##     <dbl>    <dbl> <fct>  <chr>  <chr>
##  1 -1.24  0.224    male   male   TN
##  2  0.347 0.586    female male   FN
##  3  2.14  0.895    female female TP
##  4  1.05  0.740    female male   FN
##  5 -3.89  0.0200   male   male   TN
##  6  1.11  0.751    female female TP
##  7 -8.30  0.000249 male   male   TN
##  8  2.60  0.931    female female TP
##  9 -5.34  0.00477  male   male   TN
## 10 -6.27  0.00188  male   male   TN
## # … with 323 more rows
```

```
confusion %>%
  # how many in each classif category?
  count(classif)
```

```
## # A tibble: 4 x 2
##   classif     n
##   <chr>   <int>
## 1 FN         23
## 2 FP          4
## 3 TN        164
## 4 TP        142
```

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN}$$

```
## No code, no answer:
(142 + 164) / (142 + 4 + 164 + 23)
```

```
## [1] 0.9189189
```

```r
confusion %>%
  count(classif) %>%
  pivot_wider(names_from = classif, values_from = n)
```

```
## # A tibble: 1 x 4
##      FN    FP    TN    TP
##   <int> <int> <int> <int>
## 1    23     4   164   142
```

```r
confusion %>%
  count(classif) %>%
  pivot_wider(names_from = "classif", values_from = "n") %>%
  mutate(accuracy = (TP + TN)/(TP + TN + FP + FN)) %>%
  pull(accuracy)
```

```
## [1] 0.9189189
```

How good is the model?

- In linear regression, we can gauge the model performance with R^2 and RMSE.
- In logistic regression, performance **depends** on your chosen threshold! So, how do we choose a threshold?
  - Usually, find the threshold that makes the false positive rate <5%>
- We also use **AUC** (area under the curve... what curve?)

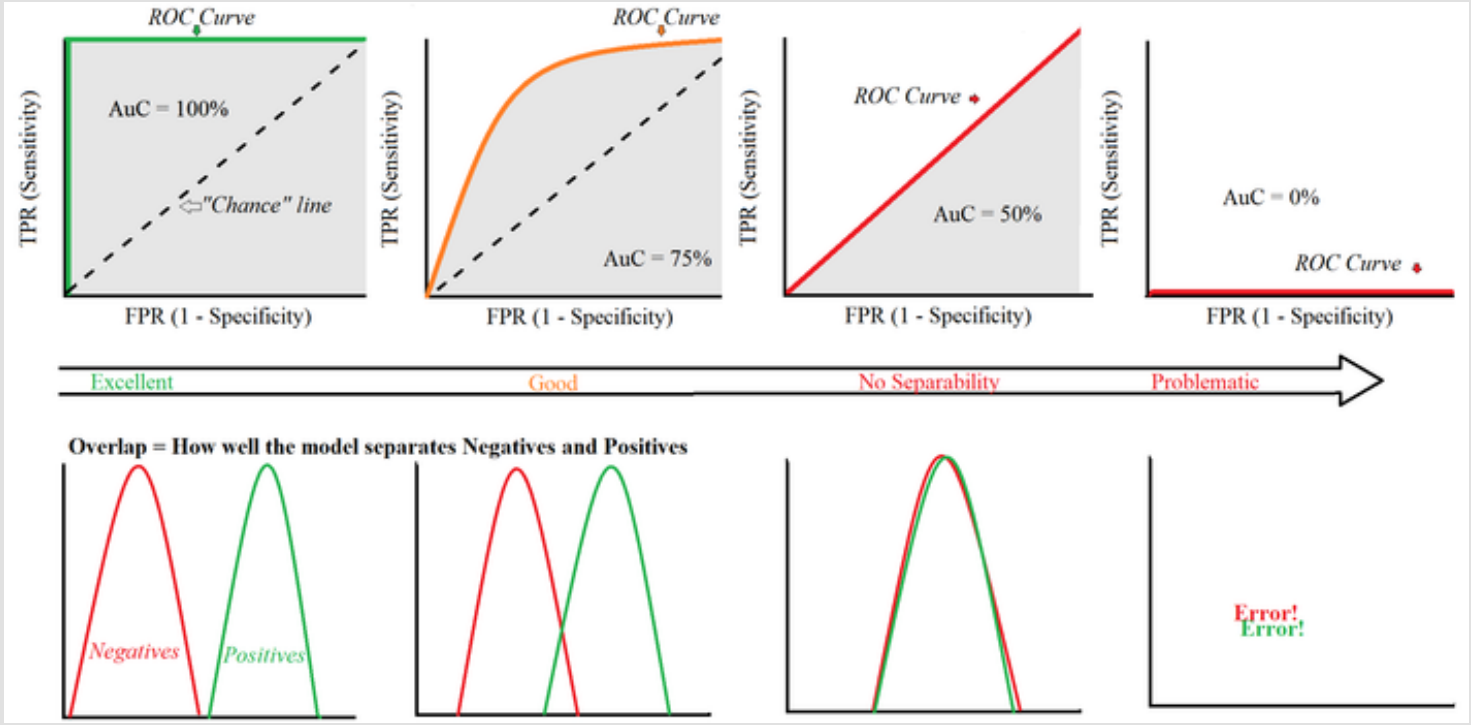
Evaluating logistic regressions

Receiver Operating Characteristic Curve

- TPR on Y-axis
- FPR (1 - specificity) on X-axis
- The AUC (**a**rea **u**nder the **c**urve) is an overall assessment of performance *at any threshold*

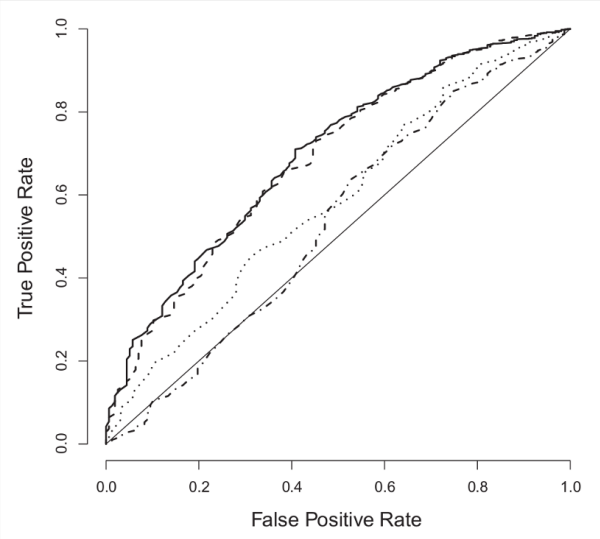
- $TPR = TP/P = \frac{TP}{TP+FN}$ (*sensitivity* AKA *recall*)
- $TNR = TN/N = \frac{TN}{FP+TN}$ (*specificity*)
- $FPR = FP/N = \frac{FP}{FP+TN}$ (*1 - specificity*)

Getting a "feel" for ROC curves

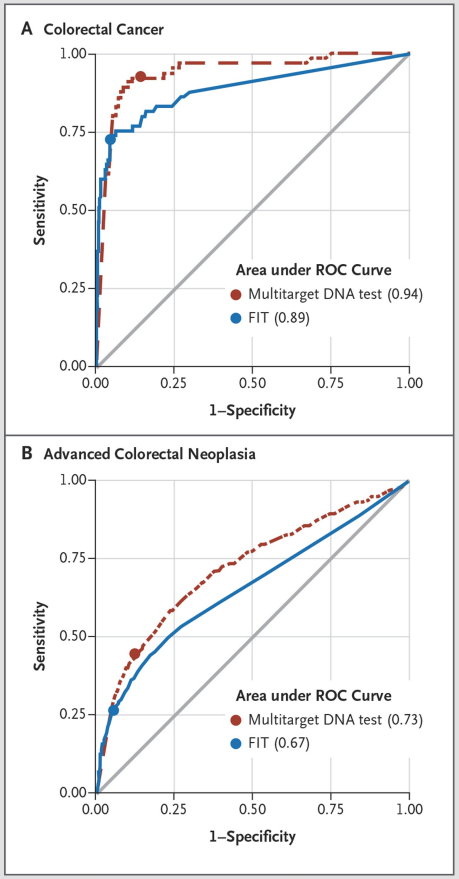


Examples of ROC curves in the literature

Keller et al. Genome Biol Evol 2012; 4:80-88



Imperiale et al. N Engl J Med 2014; 370:1287-1297



ROC vs PR

- ROC curves are suitable when data is *balanced*
  - Similar amounts of positives, negatives in the dataset
  - FPR (1 - specificity) on X-axis, TPR on Y-axis
- **Precision-Recall** curves are more suitable for *unbalanced* data
  - Precision (PPV) on Y-axis, recall (TPR) on X-axis

- $TPR = TP/P = \frac{TP}{TP+FN}$ (*recall*)
- $FPR = FP/N = \frac{FP}{FP+TN}$
- $PPV = \frac{TP}{TP+FP}$

Is the penguin data balanced? Yes.

```
peng_nona %>%
  count(sex)
```

```
## # A tibble: 2 x 2
##   sex        n
##   <fct>  <int>
## 1 female   165
## 2 male     168
```

- *Problematically imbalanced* would be 4000 females and 5 males, or vice versa.

Making ROC curves

- Recall:
  - Our model fit is saved in `fit`
  - Our model was built with `peng_nona_sex01` dataset

```
## Use the pROC library to help you - installed already in cloud!
library(pROC)
```

```
## Use the function roc()!!
model_roc <- roc(peng_nona_sex01$sex, fit$linear.predictors)

## This also works the same:
model_roc <- roc(peng_nona_sex01$sex, fit$fitted.values)
```

Getting information out

```
model_roc$auc
```

```
## Area under the curve: 0.977
```

> Models are usually **not this good.**

```
#Piped into head() to fit on the slide

## True positive rates: The x-axis!!
model_roc$sensitivities %>% head()
```

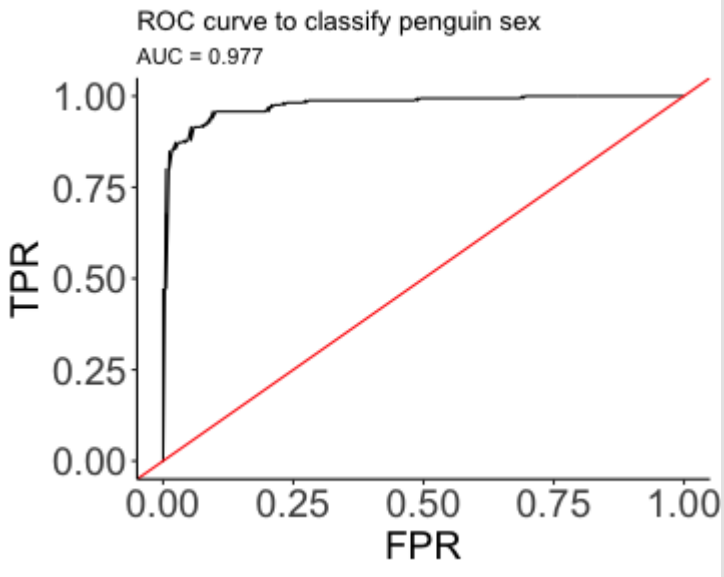
```
## [1] 1 1 1 1 1 1
```

```
## False positives rates: The y-axis!!
1 - model_roc$specificities %>% head()
```

```
## [1] 1.0000000 0.9940476 0.9880952 0.9821429 0.9761905 0.9702381
```

Make an ROC curve

```
tibble(TPR = model_roc$sensitivities,
       FPR = 1 - model_roc$specificities) %>%
  ggplot(aes(x = FPR, y = TPR)) +
  geom_line() +
  labs(title = "ROC curve to classify penguin sex",
       subtitle = paste("AUC =",round(model_roc$auc, 3)) ) +
  ## this is the y=x line to GUIDE US and help us interpret the curve
  geom_abline(col = "red")
```



Making predictions

> This is the same as running the model on new data it has never seen (this is important!)

```
## To remind you: What were the predictors?
tidy(fit)
```

```
## # A tibble: 6 x 5
##   term             estimate std.error statistic  p.value
##   <chr>               <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)      76.1       9.80         7.76 8.34e-15
## 2 speciesChinstrap  6.90      1.56         4.43 9.56e- 6
## 3 speciesGentoo     7.88      2.25         3.50 4.62e- 4
## 4 bill_len         -0.620     0.131       -4.74 2.11e- 6
## 5 bill_dep         -1.64      0.331       -4.97 6.69e- 7
## 6 mass             -0.00596   0.00106     -5.62 1.88e- 8
```

Making predictions

```
what_are_you_new_penguin <- tibble(
  species  = "Gentoo",
  bill_len = 41.5,
  bill_dep = 13.6,
  mass     = 3850
)

## NEED `type = "response"` to get a probability out
predict(fit, what_are_you_new_penguin, type = "response")
```

```
##         1
## 0.9999976
```

Validating with training/testing

```
set.seed(1) # reproducibility!!

training_frac <- 0.6

## Training and testing data splits
peng_nona_sex01 %>%
  sample_frac(training_frac) -> train_data
anti_join(peng_nona_sex01, train_data) -> test_data

## Fit to training
our_formula <- fit$call$formula # previously made!
train_fit <- glm(our_formula, data = train_data, family = "binomial")

## How's the training data model?
training_roc <- roc(train_data$sex, train_fit$fitted.values)
training_roc$auc
```

```
## Area under the curve: 0.9874
```

We have to take an extra step for logistic (vs linear) regression and fit the model to test data ourselves, since we don't have any nice `modelr` helper functions like `rsquare()` and `rmse()`.

```
## Fit the model to the testing data
test_fit <- predict(train_fit, test_data, type = "response")

## How's the testing data model?
testing_roc <- roc(test_data$sex, test_fit)
testing_roc$auc
```

```
## Area under the curve: 0.9588
```

All together now:

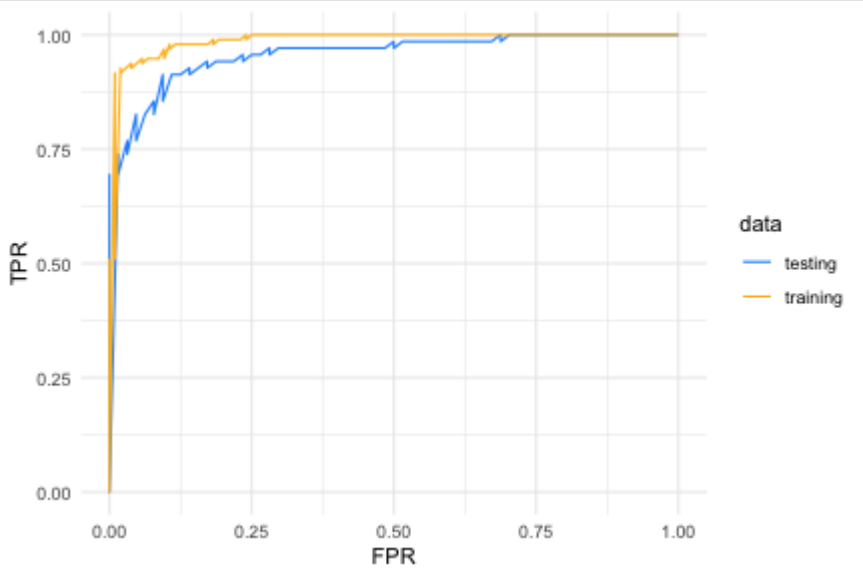
Data	AUC
Training	0.9874
Testing	0.9588

Seem this model performs pretty darn well.

One ROC curve to rule them all.

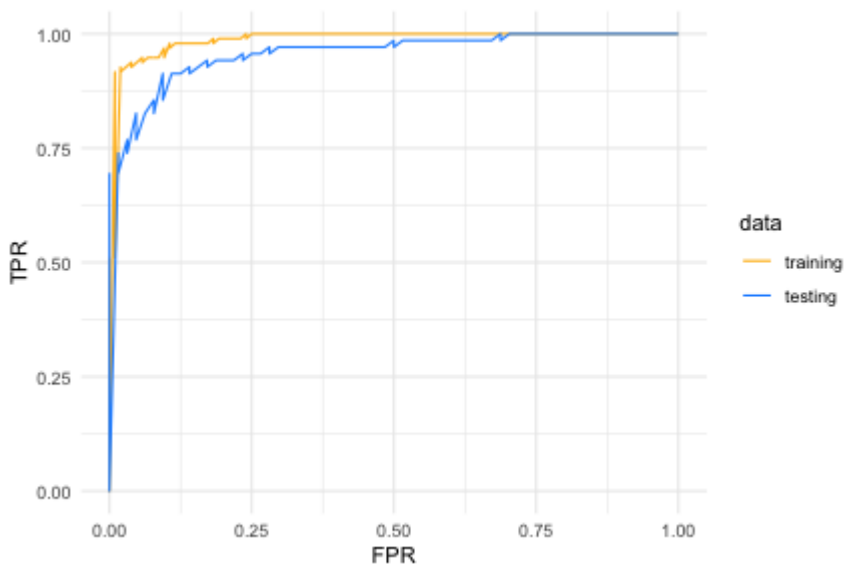
```
train_and_test <- tibble(
  TPR = c(training_roc$sensitivities, testing_roc$sensitivities),
  FPR = c(1 - training_roc$specificities, 1 - testing_roc$specificities),
  data = c(rep("training", length(training_roc$sensitivities)),
           rep("testing", length(testing_roc$sensitivities))
          )
)
```

```r
ggplot(train_and_test) +
  aes(x = FPR, y = TPR, color = data) +
  geom_line() +
  #fun!
  scale_color_manual(values = c("dodgerblue", "darkgoldenrod1")) +
  theme_minimal()
```



Don't violate best practices!

```
ggplot(train_and_test) +
  aes(x = FPR, y = TPR,
      color = fct_relevel(data, c("training", "testing"))) +
  geom_line() +
  scale_color_manual(name = "data",
                     values = c("darkgoldenrod1", "dodgerblue")) +
  theme_minimal()
```



Final words of wisdom

- Visualizing the model = the literal logistic curve
- Visualizing the model performance = ROC curve

- In the ROC curves you may have noticed a weird spike at the beginning. Don't worry about it. It's a consequence of using the pROC package.