

Lesson 12: Assessing Model Fit

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Learning Objectives

1. Use the Pearson residual statistic to determine if our preliminary final model fits the data well
2. Use the Hosmer and Lemeshow goodness-of-fit statistic to determine if our preliminary final model fits the data well
3. Use the ROC-AUC to determine how well model predicts binary outcome
4. Apply AIC and BIC as a summary measure to make additional comparisons between potential models

should be
AUC-ROC

Two classes ago: GLOW Study with interactions

- **Outcome variable:** any fracture in the first year of follow up (FRACTURE: 0 or 1)
- **Risk factor/variable of interest:** history of prior fracture (PRIORFRAC: 0 or 1)
- **Potential confounder or effect modifier:** age (AGE, a continuous variable)
- Fitted model with interactions:

$$\text{logit}(\hat{\pi}(\mathbf{X})) = \hat{\beta}_0 + \hat{\beta}_1 \cdot I(\text{PF} = \text{"Yes"}) + \hat{\beta}_2 \cdot \text{Age} + \hat{\beta}_3 \cdot I(\text{PF} = \text{"Yes"}) \cdot \text{Age}$$

$$\text{logit}(\hat{\pi}(\mathbf{X})) = -1.376 + 1.002 \cdot I(\text{PF} = \text{"Yes"}) + 0.063 \cdot \text{Age} - 0.057 \cdot I(\text{PF} = \text{"Yes"}) \cdot \text{Age}$$

- Let's say we are considering this model for our **final model**
- Today: determine the overall fit of this model

Two classes ago: Reporting results of GLOW Study with interactions

- Remember our main covariate is prior fracture, so we want to focus on how age changes the relationship between prior fracture and a new fracture!

For individuals 69 years old, the estimated odds of a new fracture for individuals with prior fracture is 2.72 times the estimated odds of a new fracture for individuals with no prior fracture (95% CI: 1.70, 4.35). As seen in [Figure 1 \(a\)](#), the odds ratio of a new fracture when comparing prior fracture status decreases with age, indicating that the effect of prior fractures on new fractures decreases as individuals get older. In [Figure 1 \(b\)](#), it is evident that for both prior fracture statuses, the predicted probability of a new fracture increases as age increases. However, the predicted probability of new fracture for those without a prior fracture increases at a higher rate than that of individuals with a prior fracture. Thus, the predicted probabilities of a new fracture converge at age [insert age here].

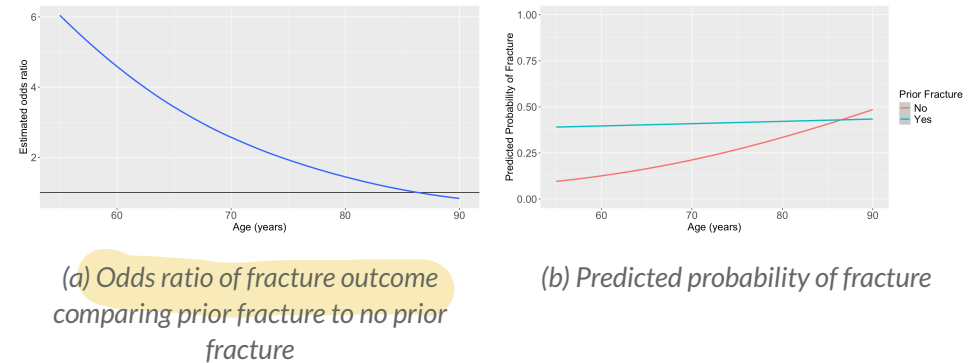


Figure 1: Plots of odds ratio and predicted probability from fitted interaction model

Assessing model fit: overview

- Once a potential final model has been determined, we need to assess the fit of the model
- Variable selection is no longer our focus at this stage
 - We want to find answer to whether the model fits the data adequately
- Assessing the Goodness of Fit or Assessing model fit
 - Assess how well our fitted logistic regression model predicts/estimates the observed outcomes
 - Comparison: fitted/estimated outcome vs. observed outcome

Some measurements for our final model(s)

- To assess the fit of the model, it is good to have a mixture of measurements

If we want to measure the absolute fit: not comparing to any models, but determining if the model fits the data well

- Pearson residual statistic
 - Not the best measurement
 - Does not work if continuous variables in model
- Hosmer-Lemeshow goodness-of-fit statistic
 - Need to adjust when sample size is large
- AUC-ROC (area under the curve of the receiver operating characteristic)

If we want comparable measures of fit: if we want to compare candidate models that are not nested

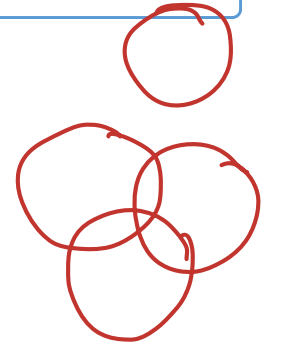
- AUC-ROC
- AIC/BIC



Variable



can use LRT

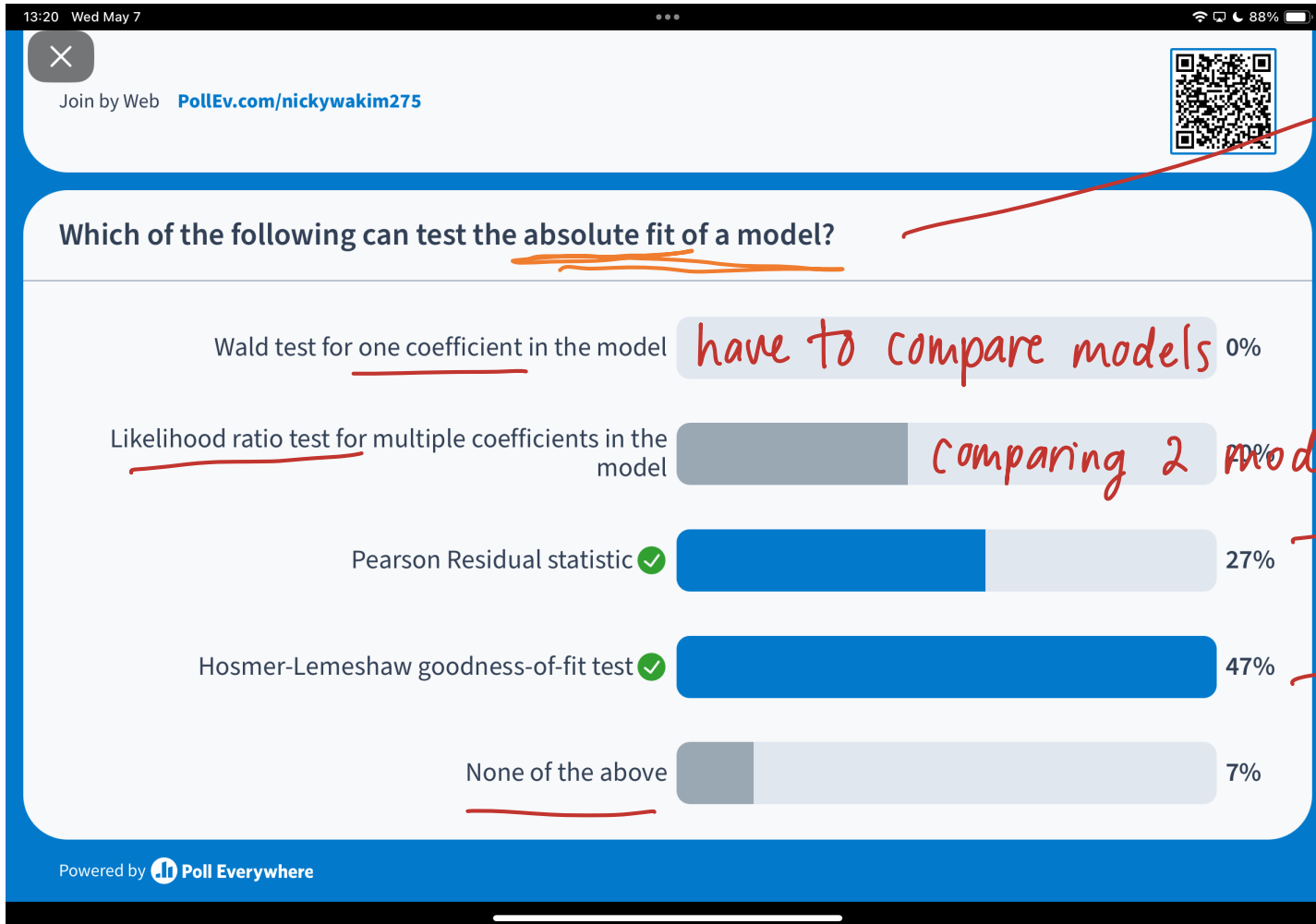


variables not
all same



cannot
use LRT

Poll Everywhere Question 1



Yes or No:
Does the model
fit the data
well?

have to compare models

comparing 2 models

test ✓

Components to Assess Model Fit

- The model fits the data well if
 - **Summary measurements of model fit** tell us good fit
 - Aka: Summary measures of the distance between the predicted/estimated/fitted and observed Y are small
 - Today's lecture!!
 - No major issues in **model diagnostics**, observations fit into model and our assumptions
 - The contribution of each pair (predicted and observed) to these summary measures is unsystematic and is small relative to the error structure of the model
 - Model Diagnostics that will be covered in another lecture!
- **Need to examine both components**
 - It is possible to see a “good” summary measure of the distance between predicted and observed Y with some substantial deviation from fit for a few subjects

Summary Measures of Goodness of Fit

- Aka overall measure of fit
- What do we need to calculate them?
 - Need to calculate the fitted outcome
 - Need to calculate how close the fitted outcome is to the observed outcome
 - Summarize across all observations (or individuals' data)
- Two tests of goodness-of-fit
 - Pearson residual statistic
 - Hosmer-Lemeshow goodness-of-fit statistic

Comparing *fitted outcome* to observed outcome

- In logistic regression model, we estimate $\pi(\mathbf{X}) = P(Y = 1|\mathbf{X})$
 - Predicted probability, $\hat{\pi}(\mathbf{X})$, is between 0 and 1 for each subject
- However, we always observe $Y = 1$ or $Y = 0$
 - Not an observed $\pi(\mathbf{X})$ *not on individual level*

- We can determine the fitted outcome by sampling Y 's from a Bernoulli distribution with the fitted probability
 - $\hat{Y} \sim \text{Bernoulli}(\hat{\pi}(\mathbf{X}))$
- If there are groups of individuals that share the *same covariate observations*, then we can use the same $\hat{\pi}(\mathbf{X})$
 - $\sum_j \hat{Y} \sim \text{Binomial}(\sum_j, \hat{\pi}(\mathbf{X}))$

- Instead of comparing the expected vs. observed at individual level, we can compare them at "group" level

Number of Covariate Patterns

- When the logistic regression model contains only categorical covariates, we can think of the number of covariate patterns
- For example:** model contains two binary covariates (history of fracture and smoking status), there will be 4 unique combination of these factors
 - This model has 4 covariate patterns
 - Subjects can be divided into 4 groups based on the covariates' values
- We can then compute the predicted number of individuals with $Y=1$ in each group, and compare that with the actual observed number of individuals with $Y=1$ in that group

	SMK	P	F	IND	SMK	PF	Y
	0	0	1	1	0	0	0
	0	1	1	2	0	1	1
	1	0	1	3	1	0	1
	1	1	1	4	1	1	0

- We don't need to sample this
- We use the expected value (mean) of the Binomial to determine the \hat{Y} for each covariate pattern
- For covariate pattern j with m_j observations:

$$\hat{Y}_j = m_j \hat{\pi}(\mathbf{X}_j) = m_j \hat{\pi}_j$$

\hat{Y}_j : expected # observations w/ $Y=1$ in cov patt j
 m_j : # of obs in cov pattern j
 $\hat{\pi}(\mathbf{X}_j)$: pred prob for cov pattern j
 $\hat{\pi}_j$: pred prob for cov pattern j

Learning Objectives

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Pearson Residual

- In logistic regression model, can use Pearson residual for summary measure of goodness-of-fit Uses the \hat{Y}_j fitted value from previous slide
- Pearson residual for j th covariate pattern is:

$$r(Y_j, \hat{\pi}_j) = \frac{(Y_j - m_j \hat{\pi}_j)}{\sqrt{m_j \hat{\pi}_j (1 - \hat{\pi}_j)}} = \frac{(Y_j - \hat{Y}_j)}{\sqrt{\hat{Y}_j (1 - \hat{\pi}_j)}}$$

- The summary statistics of Pearson residual is thus:

↳ Sum of squared Pearson resid

$$X^2 = \sum_{j=1}^J r(Y_j, \hat{\pi}_j)^2$$

sum across covariate patterns

in cov patt j:

Y_j : observed # observations w/ $Y=1$
 \hat{Y}_j = expected/pred # observations w/ $Y=1$

Pearson Residual procedure

1. Set the **level of significance** α
2. Specify the **null** (H_0) and **alternative** (H_A) **hypotheses**: same for all data
 - H_0 : model fits well **Yes**
 - H_1 : model does not fits well **No**
3. Calculate the **test statistic** and **p-value** → **Pearson resid stat**
4. Write a **conclusion** to the hypothesis test
 - Do we reject or fail to reject H_0 ?
 - Write a conclusion in the context of the problem

} Does model fit data well?

Not going to bother going through an example

- We can calculate this by hand and test against a chi-squared distribution
- No set R code to do this *
- I do not see this as the main way to determine goodness of fit... for a binary outcome!
 - Often because of the bigger issues with it... (next slide)

in ref to R fns

Issues with Pearson Residuals

- Assume current model has p covariates...
 - then χ^2 (Pearson residual) follows a chi-squared distribution
 - under the null hypothesis based on large sample theory
 - **Only appropriate if the number of covariate patterns is less than the number of observations**
- When the logistic regression model contains **one or more continuous covariates**, it is likely that the **number of covariate patterns equals to the sample size n**
- We should **not use Pearson Residuals** to evaluate goodness-of-fit test when the fitted **model contains one or more continuous variables**

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Hosmer-Lemeshow test

- If number of covariate patterns is roughly same as the number of observations
 - Whenever you include a continuous variable in your model
 - **Hosmer-Lemeshow (HL) goodness-of-fit test** should be used instead
- However, HL test does not work well if the number of covariate patterns is small
 - HL test should not be used if the number of covariate patterns ≤ 6
 - For reference: 3 binary predictors makes 8 covariate patterns
 - Pearson residuals X^2 should be used when the number of covariate patterns is small
- A large p-value from HL test suggests the model fits well

↳ H_0 : model fits well

H_1 : model does not fit well

Poll Everywhere question 2

13:47 Wed May 7

Join by Web PollEv.com/nickywakim275

Which goodness of fit test should I use to test if model with prior fracture and age fits the GLOW data well?

Pearson Residuals 13%

Hosmer-Lemeshow test 87%

Powered by Poll Everywhere

Yes/No
1/0



numeric/continuous
↳ adds a lot of covar. patterns

↳ small # cov patterns

↳ large # cov patterns

Hosmer-Lemeshow test

- HL test uses groupings from percentiles to basically measure what Pearson residual measures

- Steps to compute HL test statistic:

1. Compute estimated probability $\hat{\pi}(\mathbf{X})$ for all n subjects ($n = 1, 2, \dots, n$)

2. Order $\hat{\pi}(\mathbf{X})$ from largest to smallest values

3. Divide ordered values into g percentile grouping (usually $g = 10$ based on H-L's suggestion)

4. Form table of observed and expected counts

5. Calculate HL test statistic from table

6. Compare HL test statistic to chi-squared distribution (χ^2_{g-2})

w/in each percentile grp

*for N:
why $g-2$ df?*

Hosmer-Lemeshow test statistic

- The test statistic of Hosmer-Lemeshow goodness-of-fit test is denoted by \hat{C} , which is obtained by calculating the Pearson chi-squared statistic from the $g \times 2$ table of observed and estimated expected frequencies

$$\sum \frac{(O - E)^2}{var}$$

$$\hat{C} = \sum_{k=1}^g \frac{\overset{\text{obs\#}}{O_k} - \overset{\text{exp}}{n'_k \bar{\pi}_k}}{\underline{n'_k \bar{\pi}_k (1 - \bar{\pi}_k)}}^2$$

- where n'_k is the total number of subjects in the k th group
- Let c_k be the number of covariate patterns in the k th decile:

$$O_k = \sum_{i=1}^{n'_k} y_i \quad \leftarrow \quad O_k = \sum_{j=1}^{c_k} y_j$$

and

avg pred prob in %tile grp $\bar{\pi}_k = \sum_{j=1}^{c_k} \frac{m_j \hat{\pi}_j}{n'_k}$

g %tile grp	\hat{Y}_g pred # w/ $Y=1$	Y_g obs # w/ $Y=1$
1	10	9
2	20	18
3		
4		
5		
6		
⋮		

Hosmer-Lemeshow test procedure

1. Set the **level of significance** α

2. Specify the **null** (H_0) and **alternative** (H_A) **hypotheses**: same for all data

• H_0 : model fits well

• H_1 : model does not fits well

fail to reject if p-value ≥ 0.05
reject null if p-value < 0.05

3. Calculate the **test statistic** and **p-value**

• Note: $\hat{C} \sim \chi^2_{df=g-2}$

4. Write a **conclusion** to the hypothesis test

• Do we reject or fail to reject H_0 ?

• Write a conclusion in the context of the problem

GLOW Study: Hosmer-Lemeshow test

- Okay, so let's look at the interaction model from last class

→ PF = "Yes"

$$\text{logit}(\pi(\mathbf{X})) = \beta_0 + \beta_1 \cdot I(\text{PF}) + \beta_2 \cdot \text{Age} + \beta_3 \cdot I(\text{PF}) \cdot \text{Age}$$

↳ PF = "Yes"

- We need to fit the model and use a new command:

```
1 glow_m3 = glm(fracture ~ priorfrac + age_c + priorfrac*age_c,  
2             data = glow, family = binomial)  
3 library(ResourceSelection)  
4 obs_vals = as.numeric(glow$fracture) - 1  
5 fit_vals = fitted(glow_m3)  
6 hoslem.test(obs_vals, fit_vals, g = 10)
```

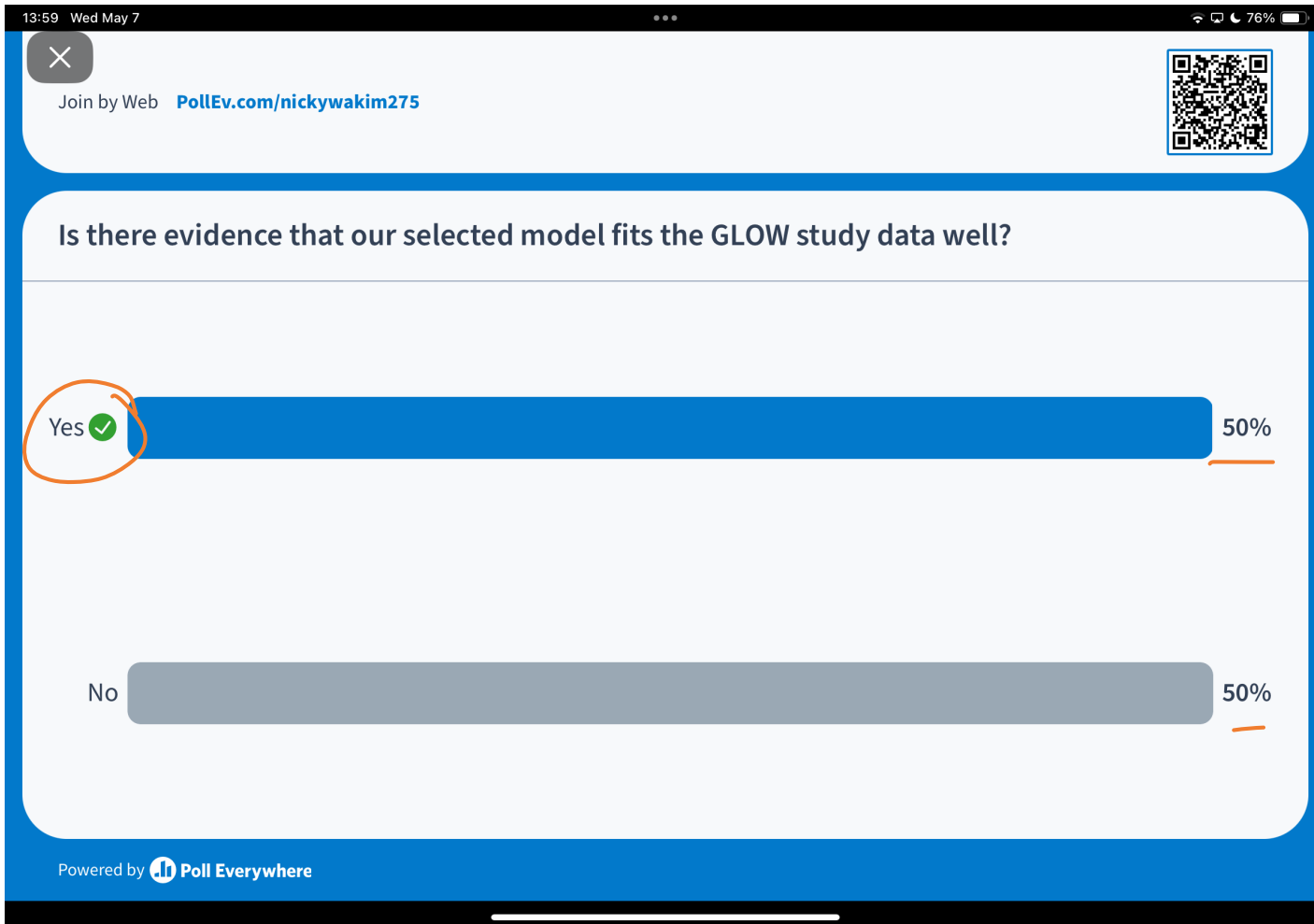
Hosmer and Lemeshow goodness of fit (GOF) test

data: obs_vals, fit_vals

X-squared = 6.778, df = 8, p-value = 0.5608 > 0.05

Note to Nicky: do NOT make conclusion yet! In the poll everywhere!

Poll Everywhere question 3



$p\text{-val} = 0.56$
 > 0.05
fail to reject
↳ model fits well.

GLOW Study: Hosmer-Lemeshow test

- Conclusion: The p-value is 0.5608, so we *fail to reject* the null hypothesis that the model fits the data well. Thus, for the GLOW study data, the model with an interaction between age and prior fracture fits the data well
- Don't forget that we still need to check individual observations (Model Diagnostics!)
- R may give results for the HL test even if it is not appropriate to use it!
 - **If number of covariate patterns ≤ 6 , do not use HL test**

Large sample size issue in H-L test

- When the sample size is really big (> 1000), it is much more likely to find the H-L reject the model fit (even when the expected vs. observed in each decile categories looks pretty similar)
- This is due to “too much” power in hypothesis testing.
 - Paul et al. (2012) for samples sizes from 1000 to 25,000, the number of groups g should be equal to

$$g = \max \left(10, \min \left\{ \frac{n_1}{2}, \frac{n - n_1}{2}, 2 + 8 \left(\frac{n}{1000} \right)^2 \right\} \right)$$

$\frac{1000}{2} = 500$ $\frac{9000}{2} = 4500$ $2 + 800 = 802$

- For example, if one has a sample with $n = 10,000$ (sample size) and $n_1 = 1,000$ (number of events) then $g = 500$ groups are suggested
- For $n > 25000$, other methods, such as partitioning data into a developmental data set (with smaller n) and a validation set

Final Notes on Pearson and HL tests

- They should not be used for variable selection
 - The likelihood ratio tests for significance of coefficients are much more powerful and appropriate (when nested)

- They are not for model comparison
 - One should **not** use the p-value from goodness of fit tests of different models to decide which model is better than the other
 - Something like AUC-ROC, AIC, or BIC can be used

Learning Objectives

1. Use the Pearson residual statistic to determine if our preliminary final model fits the data well
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ROC Curve and AUC (1/2)

- Receiver Operating Characteristics (ROC) curve is useful tool to quantify how good is our model predicting binary outcome
- It is a plot of sensitivity (true positive rate) versus (1-specificity) or false positive rate of fitted binary values

- True Positive Rate =
$$\frac{TP}{TP + FN}$$

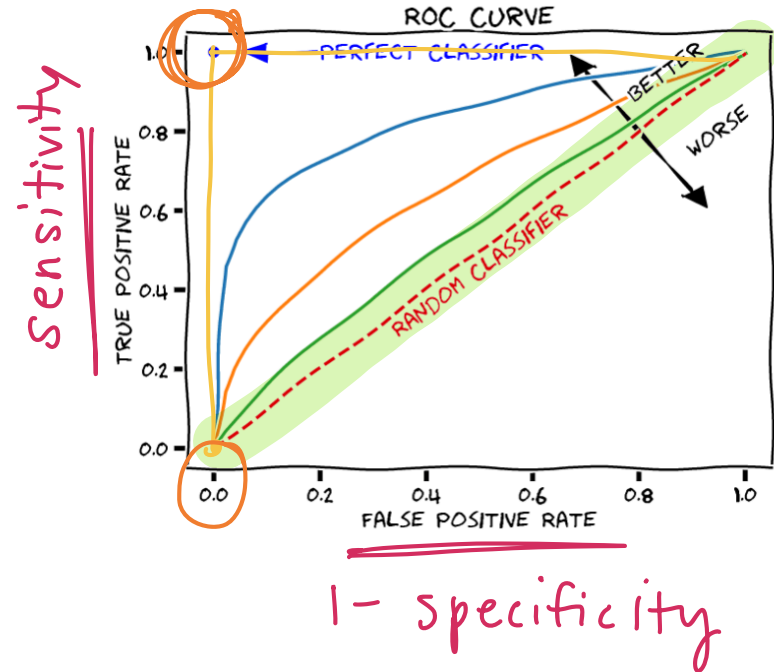
- False Positive Rate =
$$\frac{FP}{FP + TN}$$

- The ROC curve shows the tradeoff between sensitivity and specificity

		Observed outcome	
		1	0
Predicted/fitted outcome	1	TP ✓	FP ✗
	0	FN ✗	TN ✓

ROC Curve and AUC (2/2)

- Area under the ROC curve (AUC ROC) is a reasonable summary of the overall predictive accuracy of the test
 - Accuracy means how well the predicted value matches the observed value
- The closer the curve follows the left-hand border and top border of the ROC space, the more accurate the test
 - An AUC = 1 represents 100% accuracy
- The closer the curve comes to the 45-degree diagonal line, the less accurate the test
 - An AUC = 0.5 represents an unhelpful model
 - Random predictions



Poll Everywhere Question 4

14:27 Wed May 7

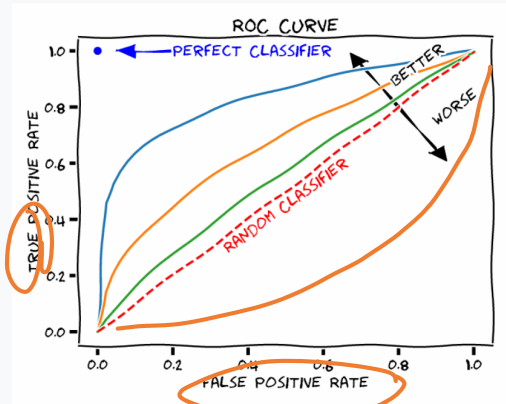
68%



Join by Web PollEv.com/nickywakim275



What does it mean if our ROC curve is below the random classifier line?



The model predicts incorrectly more often than correctly



Our model is unhelpful.



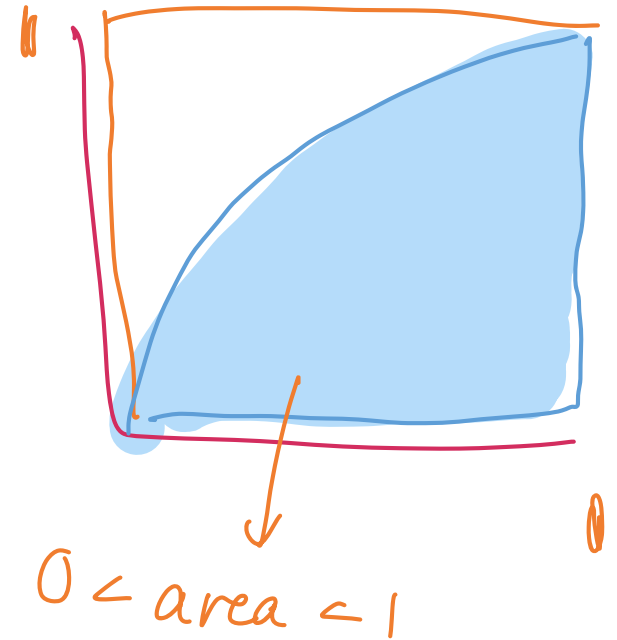
The model is actually predicting the opposite of the truth



ROC Curve and AUC (3/3)

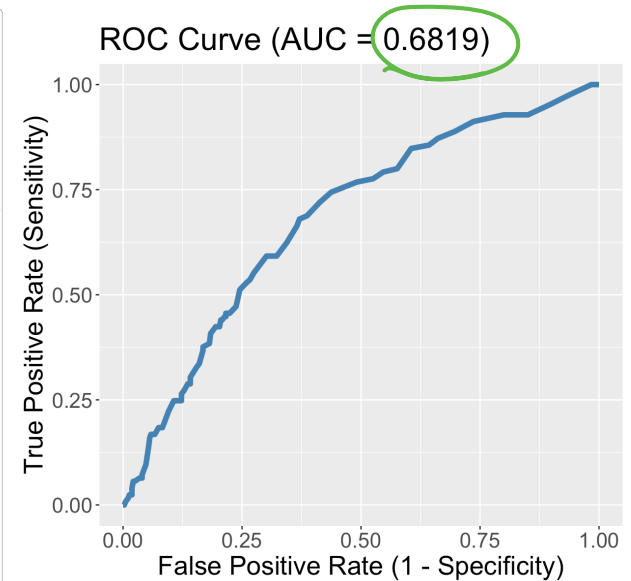
- Often only report the AUC
- Suggestions of how to interpret model fit through AUC values:

AUC Values	Fit
<u>0.5</u>	<u>Useless</u>
0.5-0.7	Poor
0.7-0.8	Acceptable
0.8-0.9	Excellent
<u>0.9-1</u>	<u>Outstanding</u>



GLOW Study: ROC of interaction model

```
1 library(pROC)
2 predicted <- predict(glow_m3, glow, type="response")
3
4 # define object to plot and calculate AUC
5 rocoj <- roc(glow$fracture, predicted) → obs, pred
6 auc <- round(auc(glow$fracture, predicted), 4)
7
8 #create ROC plot → roc() output
9 ggroc(rocoj, colour = 'steelblue',
10       size = 2, legacy.axes = TRUE) +
11 { ggtitle(paste0('ROC Curve ', '(AUC = ', auc, '')) +
12   theme(text = element_text(size = 23)) +
13   xlab("False Positive Rate (1 - Specificity)") +
14   ylab("True Positive Rate (Sensitivity)")
```



- We have a poorly fitting model
- We can take `auc` and compare it to other models: good way to pick a model based on predictive power

Another way to think about AUC

- GLOW Study: Consider the situation in which the fracture status of each individual is known
- Randomly pick one individual from fractured group and one from non-fractured outcome group
 - Based on their age and prior fracture, we will correctly predict which is from fractured group
- The AUC is the percentage of randomly drawn pairs for which we predict the pair correctly
- Therefore, AUC represents the ability of our covariates to discriminate between individuals with the outcome (fracture) and those without the outcome

Rand's index

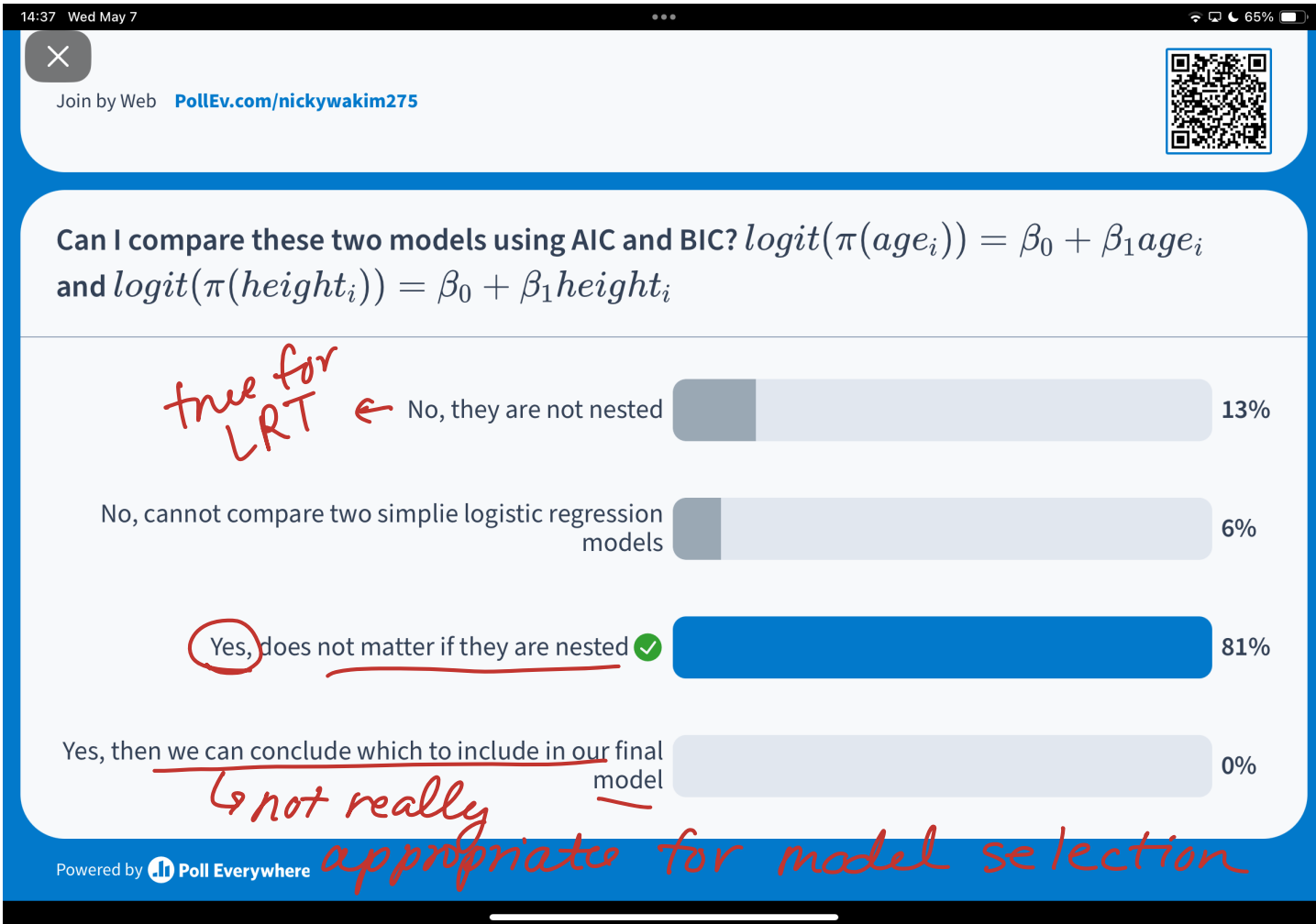
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AIC and BIC

- Two widely used non-hypothesis testing based measurements that helps select a good model
 - Akaike Information Criterion (AIC)
 - Bayesian Information Criterion (BIC)
- Unlike likelihood ratio test which is only suitable for nested model, **AIC and BIC are suitable for both nested and non-nested model**
- There is **no hypothesis/conclusion testing** for the comparison between two models
 - So not the best for selecting covariates to include in model
 - **BUT helpful if you have a few preliminary final models that you want to compare**

Poll Everywhere Question 5



AIC and BIC

- Both AIC and BIC penalize a model for having many parameters

adding penalty for q (# param in model)

Measure of fit	Equation	R code
Akaike information criterion (AIC)	$AIC = -2 \cdot \log\text{-likelihood} + 2q$	<u>AIC(model_name)</u>
Bayesian information criterion (BIC)	$BIC = -2 \cdot \log\text{-likelihood} + q \log(n)$	<u>BIC(model_name)</u>

- Where q is the number of parameters in the model and n is the sample size
- Both AIC and BIC can only be used to compare models fitting the same data set
- In comparing two models, the model with **smaller AIC and/or BIC is preferred**
 - When the difference in AIC between two models exceeds 3, the difference is viewed as “meaningful”

AIC and BIC in R

- After fitting the logistic regression model, can calculate AIC and BIC
- Let's look at the AIC and BIC of our interaction model:

```
1 AIC(glow_m3)
```

```
[1] 531.2716
```

```
1 BIC(glow_m3)
```

```
[1] 548.13
```

Example of a table for model fit statistics

```
1 model1 = glow %>% glm(formula = fracture ~ age_c + height, family = binomial)
2 model2 = glow %>% glm(formula = fracture ~ priorfrac + armassist + smoke, family = binomial)
3 model3 = glow %>% glm(formula = fracture ~ priorfrac + age_c + priorfrac*age_c, family = binomial)
4 predicted1 = predict(model1, glow, type="response")
5 predicted2 = predict(model2, glow, type="response")
6 predicted3 = predict(model3, glow, type="response")
7
8 fit_stats = data.frame(Model = c("Model 1: age + height", "Model 2: prior fracture + arm assist + smoking status", "Model 3: interaction with prior fraction + age"),
9   AUC_ROC = c(round(auc(glow$fracture, predicted1), 4), round(auc(glow$fracture, predicted2), 4), round(auc(glow$fracture, predicted3), 4)),
10  AIC = c(AIC(model1), AIC(model2), AIC(model3)),
11  BIC = c(BIC(model1), BIC(model2), BIC(model3)))
12
13 colnames(fit_stats) = c("Model", "AUC-ROC", "AIC", "BIC")
14
15 fit_stats %>% gt() %>% tab_options(table.font.size = 40) %>% fmt_number(decimals = 3)
```

Model	AUC-ROC	AIC	BIC
Model 1: age + height	0.642	542.036	554.680
Model 2: prior fracture + arm assist + smoking status	0.648	540.409	557.267
Model 3: interaction with prior fraction + age	0.682	531.272	548.130

want
highest
AUC,
lowest
AIC, BIC

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Summary (1/2)

Measure of fit	Hypothesis tested?	Equation	R code
Pearson residual	Yes	$X^2 = \sum_{j=1}^J r(Y_j, \hat{\pi}_j)^2$	Not given
Hosmer-Lemeshow test	Yes	$\hat{C} = \sum_{k=1}^g \frac{(o_k - n'_k \bar{\pi}_k)^2}{n'_k \bar{\pi}_k (1 - \bar{\pi}_k)}$	<code>hoslem.test()</code>
AUC-ROC	Kinda	Not given	<code>auc(observed, predicted)</code>
AIC	Only to compare models	$AIC = -2 \cdot \log\text{-likelihood} + 2q$	<code>AIC(model_name)</code>
BIC	Only to compare models	$AIC = -2 \cdot \log\text{-likelihood} + q \log(n)$	<code>BIC(model_name)</code>

Special notes:

- Use Hosmer-Lemeshow test over Pearson residual unless number of covariate patterns is less than 6
- Cannot use Pearson residual when there is a continuous variable in the model

Summary (2/2)

- For our interaction model:

$$\begin{aligned}\text{logit}(\hat{\pi}(\mathbf{X})) &= \hat{\beta}_0 & + \hat{\beta}_1 \cdot I(\text{PF}) & + \hat{\beta}_2 \cdot \text{Age} & + \hat{\beta}_3 \cdot I(\text{PF}) \cdot \text{Age} \\ \text{logit}(\hat{\pi}(\mathbf{X})) &= -1.376 & + 1.002 \cdot I(\text{PF}) & + 0.063 \cdot \text{Age} & - 0.057 \cdot I(\text{PF}) \cdot \text{Age}\end{aligned}$$

- We can examine the overall model fit using:
 - Not comparing to any other models:
 - Pearson residual: Not appropriate for this model
 - Hosmer-Lemeshow: $\hat{C} = 6.778$, p-value = 0.56
 - AUC-ROC: 0.6819
 - Can be used to compare to other models:
 - AUC-ROC: 0.6819
 - AIC: 531.27
 - BIC: 548.13

Reference slide

- We went over model fit statistics a little in BSTA 512/612 in [Lesson 13](#)
 - Included AIC and BIC