Lesson 12: Assessing Model Fit

Nicky Wakim

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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

Last Class: 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:

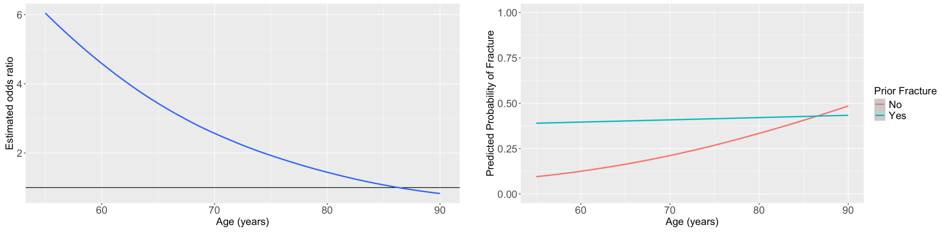
$$\begin{aligned}
\text{logit}\left(\widehat{\pi}(\mathbf{X})\right) &= \widehat{\beta}_0 && + \widehat{\beta}_1 \cdot I(\text{PF}) && + \widehat{\beta}_2 \cdot Age && + \widehat{\beta}_3 \cdot I(\text{PF}) \cdot Age \\
\text{logit}\left(\widehat{\pi}(\mathbf{X})\right) &= -1.376 && + 1.002 \cdot I(\text{PF})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

- Today: determine the overall fit of this model

Last Class: 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 predict 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].



(a) Odds ratio of fracture outcome comparing prior fracture to no prior fracture

(b) Predicted probability of fracture

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

Overview (1/2)

- 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 good measurements for our final model(s)

- Pearson residual statistic

- Hosmer-Lemeshaw goodness-of-fit statistic

- AUC-ROC (area under the curve of the receiver operating characteristic)

- AIC/BIC

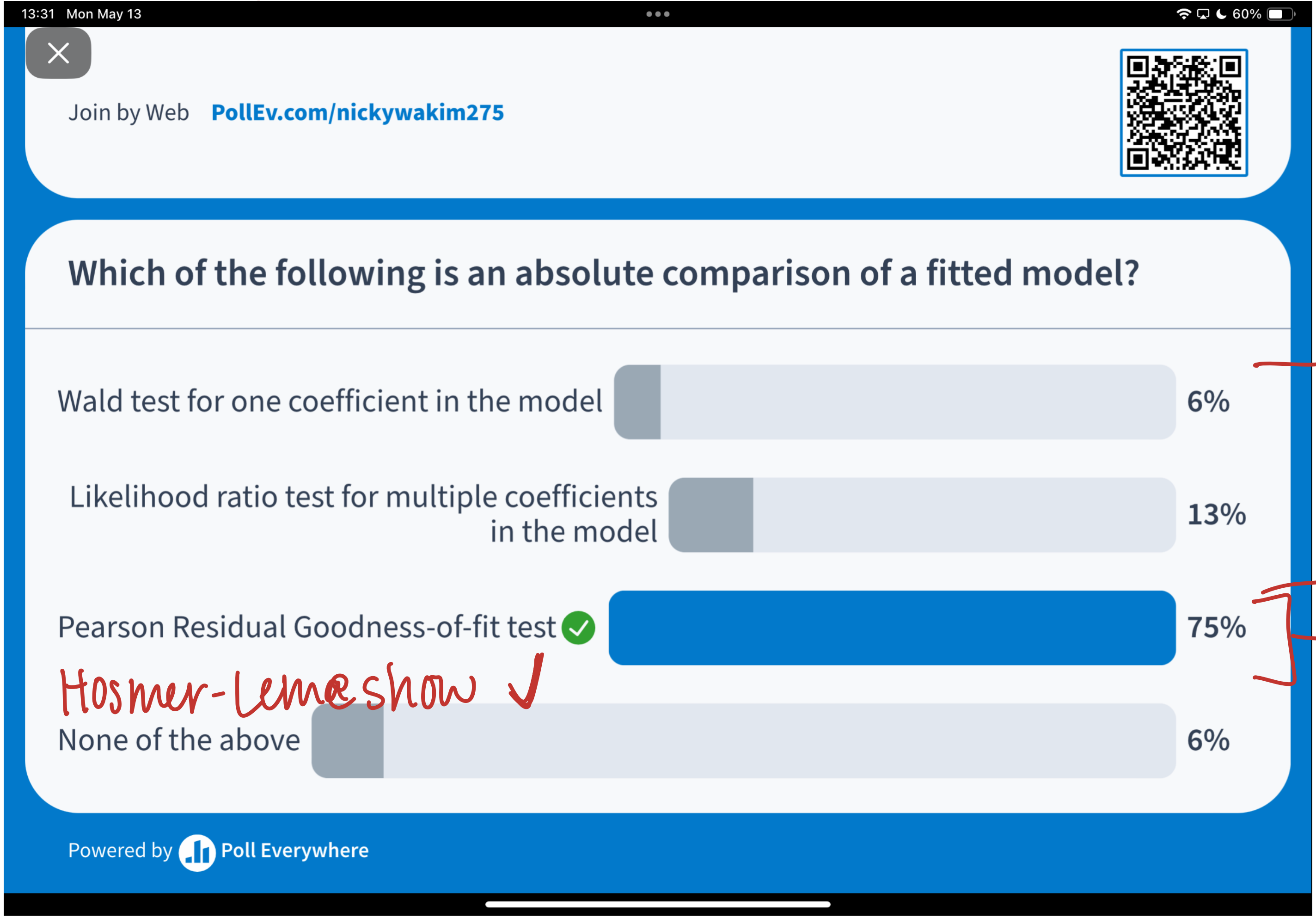
Overview (2/2)

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

- We want to **measure the absolute fit**: not comparing to any models, but determining if the model fits the data well
  - Pearson residual statistic
  - Hosmer-Lemeshaw goodness-of-fit statistic
  - AUC-ROC (kind of, often do not use a hypothesis test but you can!)

- We want **comparable measures of fit**: if we have candidate models that are not nested
  - AUC-ROC
  - AIC/BIC

Poll Everywhere Question 1



13:31 Mon May 13

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Which of the following is an absolute comparison of a fitted model?

Wald test for one coefficient in the model	6%
Likelihood ratio test for multiple coefficients in the model	13%
Pearson Residual Goodness-of-fit test ✓	75%
None of the above	6%

Hosmer-Lemeshow ✓

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variable selection

model

Components to Assess Model Fit

- The model fits the data well if
  - Summary measures of the distance between the predicted/estimated/fitted and observed Y are small
    - Today's lecture!!
  - 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 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 define what the fitted outcome is
  - 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-Lemeshaw 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 value, $\widehat{\pi}(\mathbf{X})$, is between 0 and 1 for each subject
- However, we always observe $Y = 1$ or $Y = 0$
  - Not an observed $\pi(\mathbf{X})$

$\hat{Y}$ $\hat{\pi}$

- We can deterimine the fitted outcome by sampling Y's from a Bernoulli distribution with the fitted probability
  - $\widehat{Y} \sim \text{Bernoulli}(\widehat{\pi}(\mathbf{X}))$

↳ 0, 1

- If there are groups of individuals that share the *same covariate observations*, then we can use the same $\widehat{\pi}(\mathbf{X})$
  - $\sum_j \widehat{Y} \sim \text{Binomial}(\sum_j, \widehat{\pi}(\mathbf{X}))$

for 10 ppl who have X...,
how many predicted Y=1

- 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

  $2 \times 2 = \boxed{4}$

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

10

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

10 ppl in cov pat 1

$\hat{\pi} = 0.2$

$\hat{Y} = 10 \cdot 0.2 = 2$

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Pearson Residual

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

4 groups

↓

gp 1..

$$r\left(Y_j, \hat{\pi}_j\right) = \frac{(Y_j - m_j\hat{\pi}_j)}{\sqrt{m_j\hat{\pi}_j(1-\hat{\pi}_j)}} = \frac{\overset{10 - 14}{(Y_j - \boxed{\hat{Y}_i})}}{\underline{\sqrt{\hat{Y}_i(1-\hat{\pi}_j)}}} \; 1$$

$\hat{Y} = \Sigma$ of 0 & 1

- The summary statistics of Pearson residual is thus:

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

↑

j=1 to 4

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 → want a higher p-value
   - H_1: model does not fits well
3. Calculate the **test statistic** and **p-value**
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

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…

Issues with Pearson Residuals

- Assume current model has p covariates…
  - then X^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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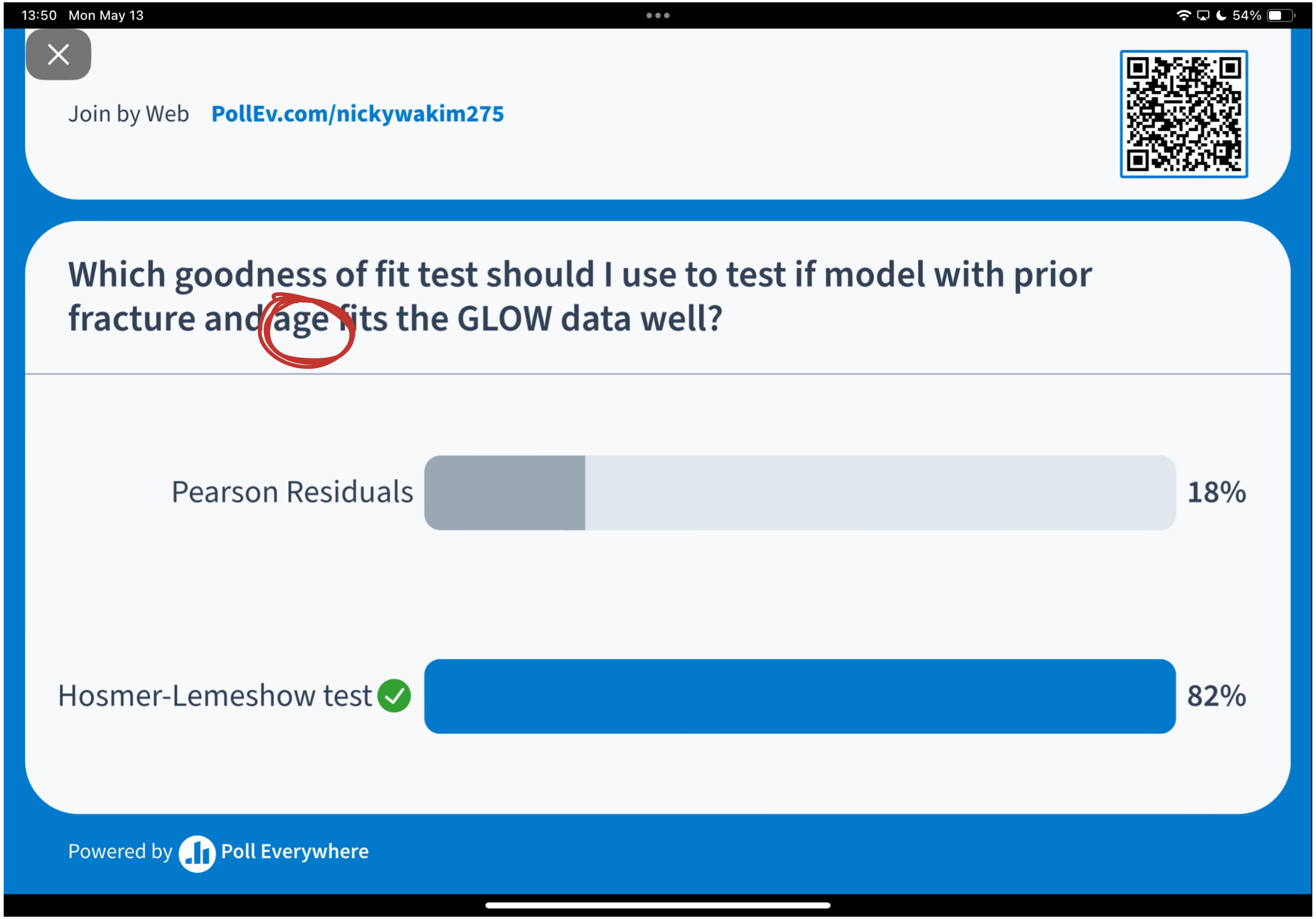
Hosmer-Lemeshow test

- 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

Poll Everwhere question 2



13:50 Mon May 13
54%
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Which goodness of fit test should I use to test if model with prior fracture and age fits the GLOW data well?

Pearson Residuals 18%

Hosmer-Lemeshow test ✓ 82%

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 $\widehat{\pi}(\mathbf{X}))$ for all n subjects $(n = 1, 2, \ldots, n)$
2. Order $\widehat{\pi}(\mathbf{X})$ 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})

Hosmer-Lemeshow test statistic

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

$$\hat{C} = \sum_{k=1}^{g} \frac{(o_k - n'_k \bar{\pi}_k)^2}{n'_k \bar{\pi}_k (1 - \bar{\pi}_k)}$$

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

$$o_k = \underline{\sum_{j=1}^{c_k} y_j} \quad \text{\# of } Y=1 \text{ w/in grp } k$$

and

$$\bar{\pi}_k = \sum_{j=1}^{c_k} \frac{m_j \hat{\pi}_j}{n'_k}$$

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
3. Calculate the **test statistic** and **p-value**
   - Note: $\underline{\widehat{C} \sim \chi^2_{df=g-2}}$
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

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

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

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

predict probs

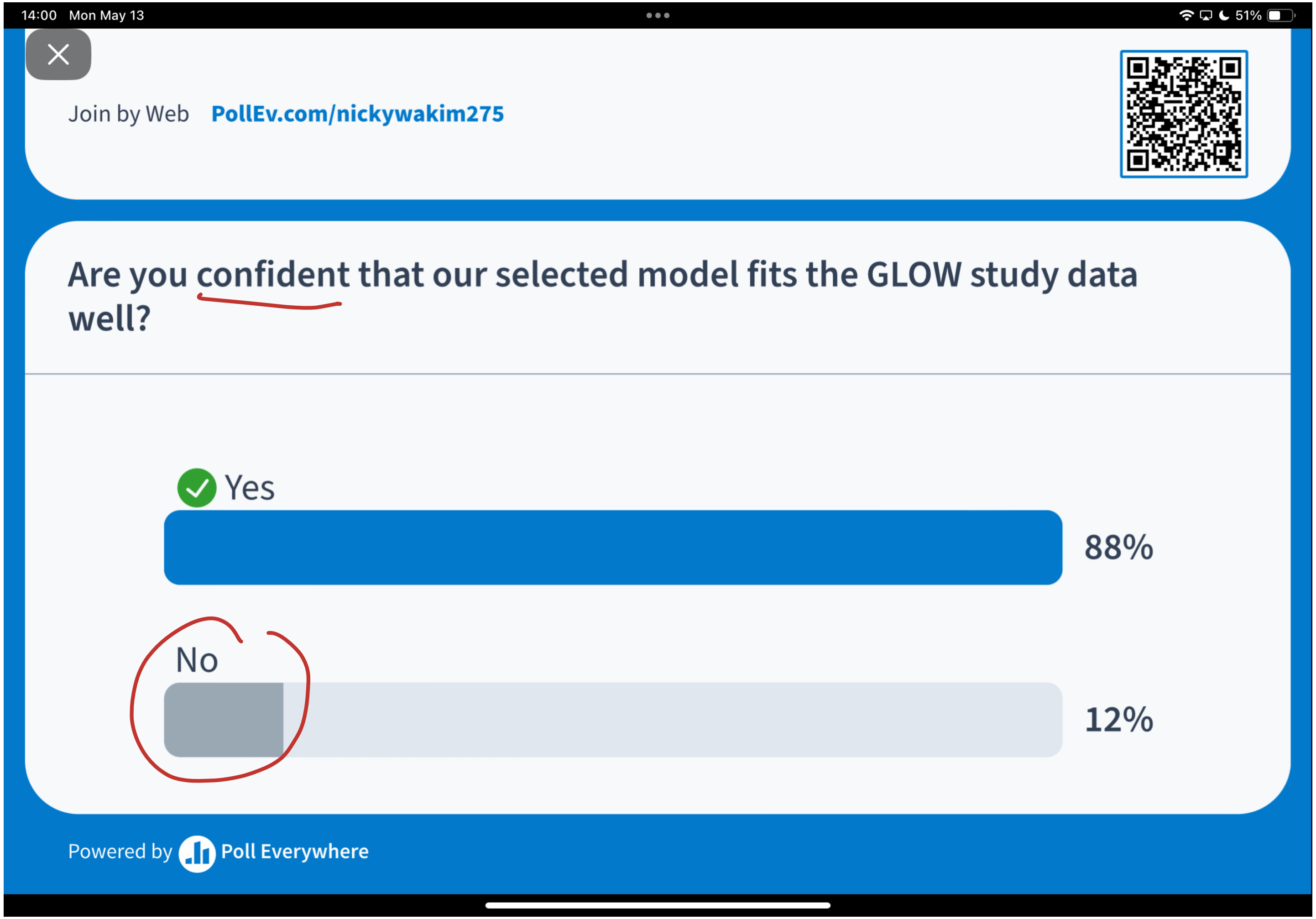
```
    Hosmer and Lemeshow goodness of fit (GOF) test

data:  obs_vals, fit_vals
X-squared = 6.778, df = 8, p-value = 0.5608
```

conclude model fits
data well

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

Poll Everywhere question 3



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51%

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Are you confident that our selected model fits the GLOW study data well?

✓ Yes — 88%

[✓ No] — 12%

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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, the ~~preliminary final~~ interaction model for the GLOW dataset 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

Big Data Issue in Goodness-of-fit 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

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

n_1 = # of outcome events/Successes

- 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

$\frac{}{2} = 500$

- For n > 25000, other methods, such as partitioning data into a developmental data set (with smaller n) and a validation set

Final Notes on Goodness-of-fit Test

- 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

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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 $= \dfrac{TP}{TP + FN}$
    - False Positive Rate $= \dfrac{FP}{FP + TN}$

- The ROC curve shows the tradeoff between sensitivity and specificity

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

specficity = true negative rate

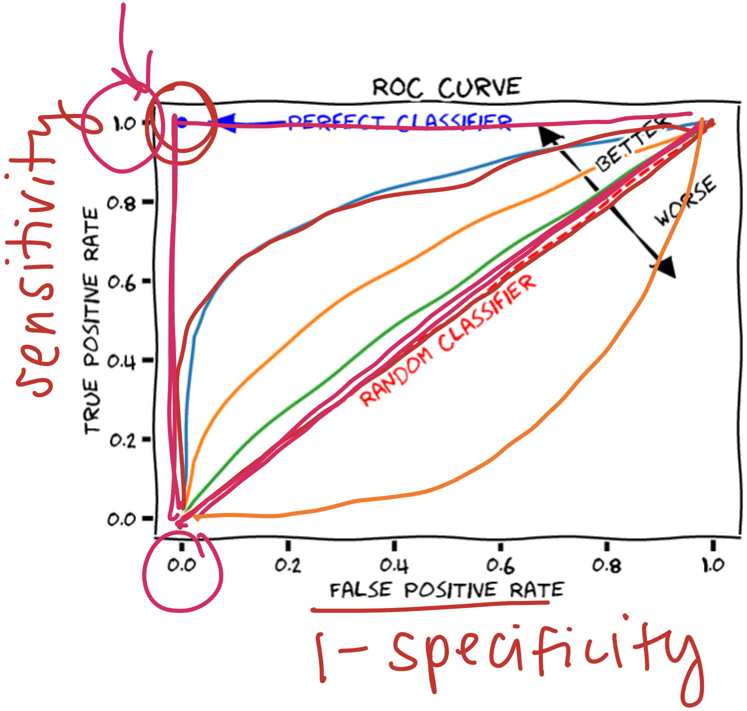
$$= \frac{TN}{FP + TN}$$

ROC Curve and AUC (2/2)

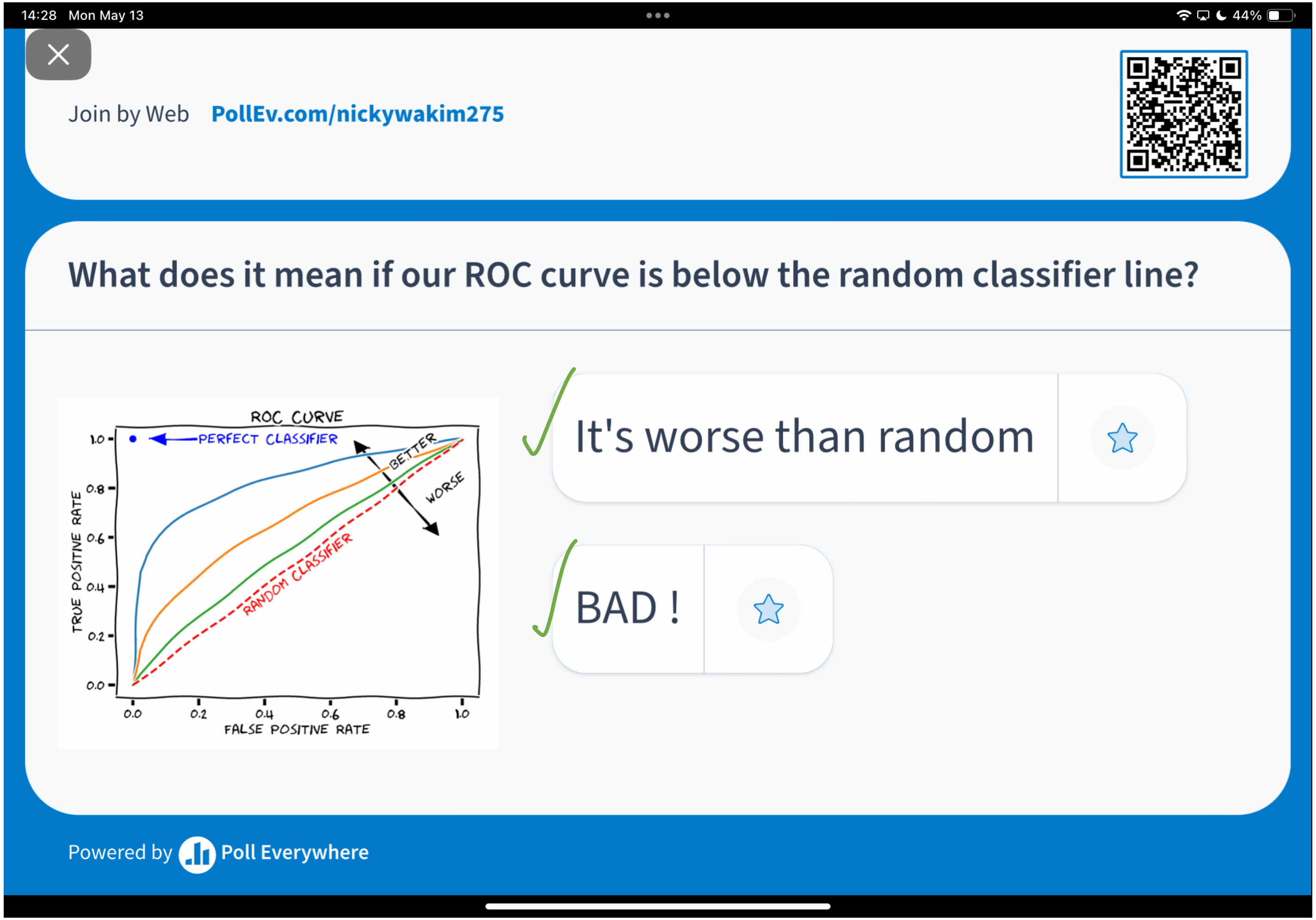
- Area under the ROC curve (AUC ROC) is a reasonable summary of the overall predictive accuracy of the test
  - Accuracy means how well the predicted value matches the observed value

- 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



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

✓ It's worse than random

✓ BAD !

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ROC Curve and AUC (3/3)

- Often only report the AUC

- Suggestions of how to interpret model fit through AUC values:

AUC Values	Fit
0.5	Uselesss
0.5-0.7	Poor
0.7-0.8	Acceptable
0.8-0.9	Excellent
0.9-1	Outstanding

GLOW Study: ROC of interaction model

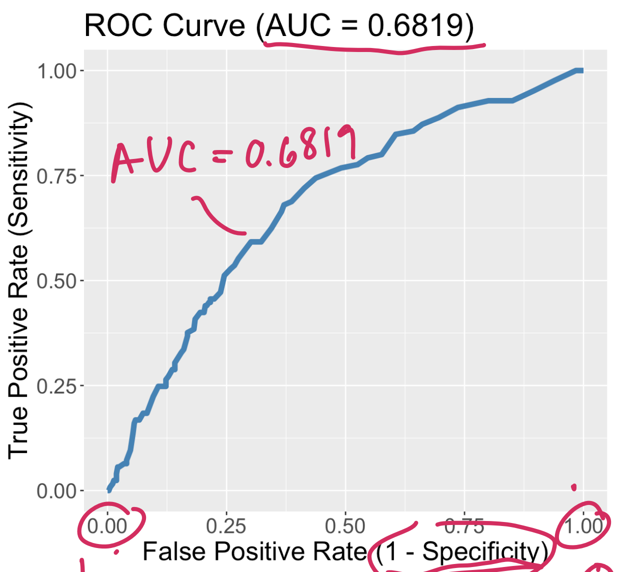
```r
library(pROC)
predicted <- predict(glow_m3, glow, type="response")

# define object to plot and calculate AUC
rocobj <- roc(glow$fracture, predicted)
auc <- round(auc(glow$fracture, predicted),4)

#create ROC plot
ggroc(rocobj, colour = 'steelblue',
        size = 2, legacy.axes = TRUE) +
  ggtitle(paste0('ROC Curve ', '(AUC = ', auc, ')')) +
  theme(text = element_text(size = 23)) +
  xlab("False Positive Rate (1 - Specificity)") +
  ylab("True Positive Rate (Sensitivity)")
```

prob

obs



1

0

specifity

- 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, ~~height~~, prior fracture, ~~and all other covariates~~, 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

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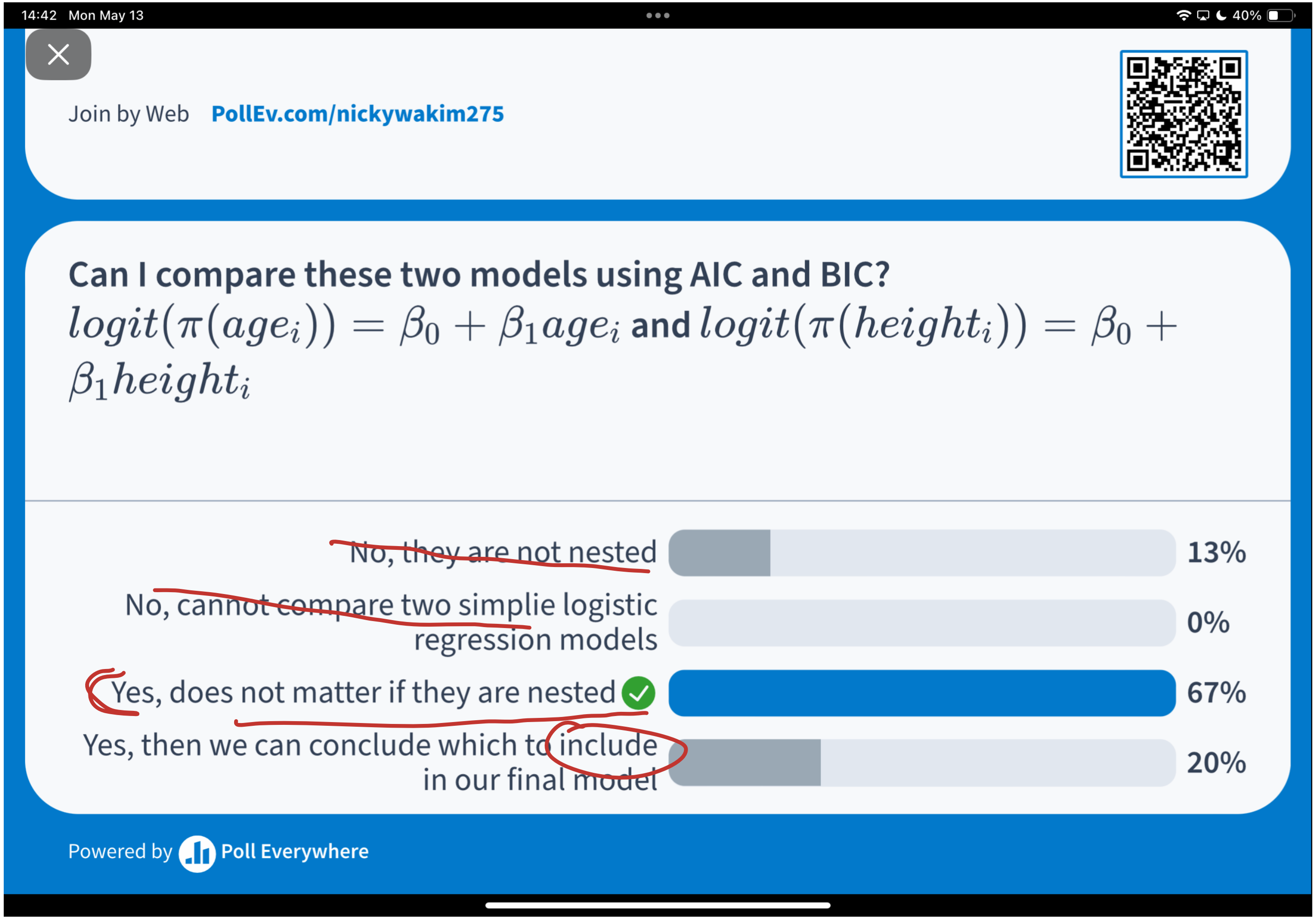
AIC and BIC

- 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



14:42 Mon May 13 40%

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Can I compare these two models using AIC and BIC?
$logit(\pi(age_i)) = \beta_0 + \beta_1 age_i$ and $logit(\pi(height_i)) = \beta_0 + \beta_1 height_i$

~~No, they are not nested~~	13%
~~No, cannot compare two simplie logistic regression models~~	0%
Yes, does not matter if they are nested ✓	67%
Yes, then we can conclude which to include in our final model	20%

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AIC and BIC

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

Measure of fit	Equation	R code
Akaike information criterion (AIC)	$AIC = \underline{-2 \cdot \text{log-likelihood}} + \boxed{2q}$	`AIC(model_name)`
Bayesian information criterion (BIC)	$\overset{B}{A}IC = \underline{-2 \cdot \text{log-likelihood}} + \boxed{q\log(n)}$	`BIC(model_name)`

- 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:

```r
AIC(glow_m3)
```

```
[1] 531.2716
```

```r
BIC(glow_m3)
```

```
[1] 548.13
```

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Summary (1/2)

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

Special notes:

- Use Hosmer-Lemshow 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:

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

- 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

	AUC	AIC	BIC
Model 1	—	—	—
Model 2	—	-	—