#### POLS/CS&SS 503: Advanced Quantitative Political Methodology

#### MODEL SPECIFICATION AND FIT

May 12, 2015

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#### Overview

### Measures of Fit $R^2$ Standard Error of the Regression Information Criteria Out-of-Sample and Cross-Validation Method

General Advice on Model Selection

## How To Choose Among Different Models?

- Depends on your purpose
- Some tools
  - · Internal model validation: residuals, outliers
  - Overall model Fit statistics: out of sample is preferred

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#### Measures of Model Fit

Various measure of how the model fits the data, both *in-sample* and *out-of-sample* 

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Standard Error of the Regression Information Criteria Out-of-Sample and Cross-Validation Metho

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## The Coefficient of Determination, $R^2$

$$\begin{split} R^2 &= \frac{\text{Explained sum of squares}}{\text{Total sum of squares}} = 1 - \frac{\text{Residual sum of squares}}{\text{Total sum of squares}} \\ &= \frac{\sum (\hat{y} - \bar{y})^2}{\sum (\hat{y} - \bar{y})^2} \\ &= 1 - \frac{\sum \hat{\epsilon}^2}{\sum (\hat{y} - \bar{y})^2} \end{split}$$

- Commonly used
- Ranges between
- Why can it never be less than 0?
- What happens when you add a variable?
- What is the case when  ${\cal R}^2=1$
- Bivariate case:  $Cor(y, x)^2$
- + General case:  $\mathrm{Cor}(y,\hat{y})^2$

# What $R^2$ does and doesn't say

- · Indirectly reports scatter around the regression line
- Only in sample
- Maximizing  $\mathbb{R}^2$  perverse:
  - Not usually interesting for explanation.  $\boldsymbol{Y}$  regressed on itself, vote choice on vote intention.
  - Not usually best for prediction
- Not an estimate

# $R^2$ varies between samples



 $R^2$  of samples drawn from a linear model with a population  $R^2 = 0.5$ .

# $\mathbb{R}^2$ is a function of variation in X



- Complete sample (red + blue):  $R^2=0.72$ ,  $\hat{\sigma}=0.65$
- Restricted sample (blue only):  $R^2=0.29$ ,  $\hat{\sigma}=0.66$

# Adjusted $R^2$ What's adjusted?

$$\begin{split} \tilde{R}^2 &= 1 - \frac{S_E^2}{S_Y^2} \\ &= 1 - \frac{n-1}{n-k-1} \times \frac{RSS}{TSS} \end{split}$$

- Where n is number of obs, k is number of variables.
- Unlike  $R^2$ , treat squared error terms as estimates of populatio, not sample statistics.
- How adjusted  $R^2$  change with respect to n? With respect to k?
- But it is an ad hoc adjustment

#### Measures of Fit



#### Standard Error of the Regression

Information Criteria Out-of-Sample and Cross-Validation Method

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## Standard Error of the Regression

The standard error of the regression is the estimate of the population  $\sigma$ :

$$\hat{\sigma}_{\epsilon} = S_E = \sqrt{\frac{\sum E_i^2}{n-k-1}} = \sqrt{\frac{\sum_i (y_i - \hat{y}_i)^2}{n-k-1}}$$

- +  $S_E$  is at least as useful to report as  $R^2$
- $S_E$ : on average, how much does the fitted value miss the actual value.
- On the same scale as *y*. Easier for interpretation and substantive importance.

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## **Likelihood Function**

- Likelihood is the probability of observing the data given a statistical model.
- The **likelihood** of a linear model with normal errors:

$$\begin{split} L(\hat{\beta}, \hat{\sigma}_{\epsilon}) &= p(y|\hat{\beta}, \hat{\sigma}) = \prod_{i} N(y_{i}|X_{i}\hat{\beta}, \hat{\sigma}_{\epsilon}^{2}) \\ &= \left(\frac{1}{\hat{\sigma}_{\epsilon}\sqrt{2\pi}}\right)^{n} \prod_{i} \exp\left(-\frac{(y_{i} - x_{i}'\hat{\beta})^{2}}{2\hat{\sigma}_{\epsilon}^{2}}\right) \\ &= \left(\frac{1}{\hat{\sigma}_{\epsilon}\sqrt{2\pi}}\right)^{n} \prod_{i} \exp\left(-\frac{\hat{\epsilon}_{i}^{2}}{2\hat{\sigma}_{\epsilon}^{2}}\right) \end{split}$$

• For computational stability (the product of probabilities is a small number), the **log likelihood** is usually used

$$\log L(\hat{\beta}, \hat{\sigma}_{\epsilon}) = -n \log \hat{\sigma}_{\epsilon} - \frac{1}{2} \log 2\pi - \frac{1}{2 \hat{\sigma}_{\epsilon}^2} \sum_i \hat{\epsilon}_i^2$$

## Information Criteria

- · Information criteria include log Likelihod + a penalty for complexity
- The two Most common are AIC and BIC:

$$\begin{split} AIC &= -2\log L(\hat{\beta}, \hat{\sigma}_{\epsilon}) + 2k\\ BIC &= -2\log L(\hat{\beta}, \hat{\sigma}_{\epsilon}) + k\log n \end{split}$$

- Lower is better
- Smaller values = better fit
- See Fox for justifications
- AIC = approx leave one out cross-validation; BIC = a specific k-fold cross-validation

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#### **Out of Sample Methods**

- Compare models on how well they do on data that was not used to estimate their parameters.
- In practice, serves as a good check against spurious findings
- Even if our goal is explanation, not prediction, scientific models strive for generality
- Usual caveat: best fitting may not be the only criteria for the model

## Out of Sample Goodness of Fit

- Method
  - 1. Split data into training  $(X_{\text{training}}, y_{\text{training}})$ , test data,  $(X_{\text{test}}, y_{\text{test}})$ .
  - 2. Fit model to training data,  $(X_{\text{training}}, y_{\text{training}})$ , obtain  $\hat{eta}_{\text{training}}$
  - 3. Calcuate fitted  $\hat{y}_{\text{test}}$  for the test sample  $(X_{\text{test}}, y_{\text{test}})$ .
  - 4. Calculate predicted mean squared error of the test data

$$RMSE_{\text{prediction}} = \hat{\sigma}_{\text{test}} = \sqrt{\frac{1}{n_{\text{test}}}\sum_{i \in \text{test}} \hat{\epsilon}_i^2}$$

- Usually MSE of test data lower than MSE of training data. In-sample fit statistics are overly optimistic.
- Good rule of thumb: 70-75% training, 30-25% test
- · Can use other prediction statistics to evaulate models

## **Cross Validation**

Reuse data for multiple in-sample and out-of-sample tests. More efficient use of data.

- + k-fold cross validation
  - 1. Select all but 1/kth of the data:  $(y_{\text{training}}, X_{\text{training}})$
  - 2. Repeat out of sample tests k times
- Leave-one-out (LOO-CV): k = n.
- 5– or 10–fold cross-validation; generally the best in terms of bias / variance tradeoff.
- The best model minimizes prediction RMSE
- **Important:** the test and trainining data should be from same "population". Randomly sampled in cross-section. Need to be careful in panel, blocked, or time-series.

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## Fox on Model Selection

#### Problems

- Simultaneous inference
- Fallacy of affirming the consequent
- Impact of large samples on hypothesis tests
- Exaggerated precision

## Fox on Model Selection

Strategies

- · Alternative model-selection criteria (not stat sig)
- Compensating for simulaneous inference
- Avoiding model selection: maximally complex and flexible model.
- Model averaging: select many models.

## Fox on Model Selection

General Advice

- It is problematic to use stat. hypoth. tests for model selection.
  Simultaneous inference, biased results. Complicated models in large *n*, exaggerated prediction. (p. 6008)
- Most methods maximize *predication* not interpretation
- When purpose is interpretation, simplify based on substantive considerations, even if that includes removing small, but stat sig coefficients. (p. 622)
- validation: using separate model choice and inference

# Gelman and Hill's Rules for Building a Regression Model for Prediction

- Include all input variables expected to be important in predicting outcome (substantively)
- Not always necessary to include these separately, e.g. indices
- · For inputs with large effects, consider including interactions
- Whether to exclude a varaible from prediction based on significance
  - Not stat sig, expected sign: keep. Will not help much, but will not hurt predictions.
  - Not stat sig, not expected sign: consider removing
  - Stat sig, not expected sign: Think hard Are there lurking variables?
  - Stat sig, expected sign: keep
- Think hard before the model; but adjust to new information
- Gelman and Hill use *predictaion* differently than Fox.

Gelman and Hill, p. 69

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#### References

- John Fox, *Applied Regression Analysis and Generalized Linear Models*, Ch. 22, "Model Selection, Averaging, and Validation".
- Christopher Adolph (Spring 2014) "Linear Regression: Specification and Fitting" [Lecture slides].

http://faculty.washington.edu/cadolph/503/topic5.pw.pdf|.