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

## MODEL SPECIFICATION AND FIT

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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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# The Coefficient of Determination, $R^2$

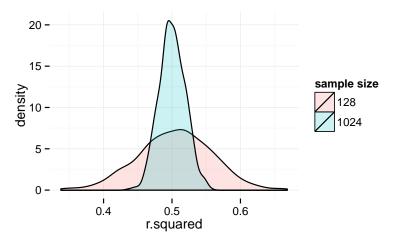
$$\begin{split} R^2 &= \frac{\text{Explained sum of squares}}{\text{Total sum of squares}} = 1 - \frac{\text{Residual sum of squares}}{\text{Total sum of squares}} \\ &= \frac{\sum (\hat{y} - \bar{y})^2}{\sum (\hat{y} - \bar{y})^2} \\ &= 1 - \frac{\sum \hat{\epsilon}^2}{\sum (\hat{y} - \bar{y})^2} \end{split}$$

- · 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:  $Cor(y, \hat{y})^2$

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

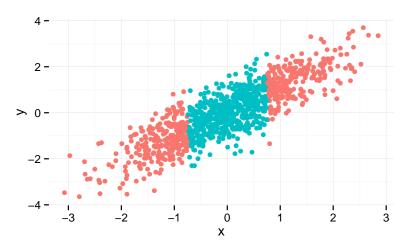
- Indirectly reports scatter around the regression line
- Only in sample
- Maximizing  $\mathbb{R}^2$  perverse:
  - Not usually interesting for explanation.  ${\cal Y}$  regressed on itself, vote choice on vote intention.
  - Not usually best for prediction
- · Not an estimate

# $\mathbb{R}^2$ varies between samples



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

## $\mathbb{R}^2$ 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?

$$\tilde{R}^2 = 1 - \frac{S_E^2}{S_Y^2}$$

$$= 1 - \frac{n-1}{n-k-1} \times \frac{RSS}{TSS}$$

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

 $R^2$ 

#### Standard Error of the Regression

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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.
- ullet On the same scale as y. Easier for interpretation and substantive importance.

 $R^2$ 

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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  $(X_{\mathsf{training}}, y_{\mathsf{training}})$ , test data,  $(X_{\mathsf{test}}, y_{\mathsf{test}})$ .
  - 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

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

- 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:  $(y_{\mathrm{training}}, X_{\mathrm{training}})$
  - 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.

 $R^2$ 

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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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- 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|.