## Linear Regression Models P8111

Lecture 15

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### Today's Lecture

- Welcome back!!
- Model selection vs. model checking
- Stepwise model selection
- Criterion-based approaches

## Model selection vs. model checking

In a model of the form

$$y|\mathbf{x} = f(\mathbf{x}) + \epsilon$$

model selection focuses on how you construct  $f(\cdot)$ ; model checking asks whether the  $\epsilon$  match the assumed form.

Things to keep in mind

- Why am I building a model?
- Is this my primary or secondary analysis?
- What predictors will I allow?
- What forms for f(x)?

### Motivation

Why am I building a model?

- Estimate associations between *x* and *y*
- Test significance of association between *x* and *y*
- Predict future *y* for new *x*

These goals will generally not result in the same final model.

## Primary vs secondary

Is this my primary or secondary analysis?

- Seriously have you (or anyone else) analyzed this data before?
- Primary analyses are often very constrained or have the goal of confirming a hypothesis
- Secondary analyses are often less constrained; may be examining hunches or generating new hypotheses

Both are valid, but have different implications for multiple comparisons

What predictors will I allow? What forms for f(x)?

 All variables? All continuous variables? Binary versions of continuous variables? Known significant variables?

Linear models? Non-linearity? Interactions?
 Some of this you know ahead of time, some you discover as you go

### Model selection is hard

- If we're asking which is the "true" model, we're gonna have a bad time
- In practice, issues with sample size, collinearity, and available predictors are real problems
- It is often possible to differentiate between better models and less-good models, though

### Estimating associations

- We may not care about whether an association is significant in our data; we're just looking for associations
- Some covariates should be included regardless of significance – models have to be convincing in the scientific context
- This can affect the baseline model, or at least the class of models one considers

### Basic idea for model selection

- Specify a class of models
- Define a criterion to summarize the fit of each model in the class
- Select the model that optimizes the criterion you're using

Again, we're focusing on f(x) in the model specification. Once you've selected a model, you should subject it to regression diagnostics – which might change or augment the class of models you specify or alter your criterion. Some examples of classes of models:

- Linear models including all subsets of *x*<sub>1</sub>, ..., *x*<sub>*p*</sub>
- Linear models including all subsets of x<sub>1</sub>, ..., x<sub>p</sub> and their first order interactions
- All functions  $f(x_1)$  such that  $f''(x_1)$  is continuous
- Additive models of the form  $f(x) = f_1(x_1) + f_2(x_2) + f_3(x_3)...$  where  $f_k''(x_k)$  is continuous

## Popular criteria

- Akaike Information Criterion
- Bayes Information Criterion
- *F* or *t*-tests
- Prediction RSS (PRESS) or CV

## Sequential methods (Forward Stepwise)

- Start with "baseline" (usually intercept-only) model
- For every possible model that adds one term, evaluate the criterion you've settled on
- Choose the one with the best "score" (lowest AIC, smallest p-value)
- For every possible model that adds one term to the current model, evaluate your criterion
- Repeat until either adding a new term doesn't improve the model or all variables are included

## Sequential methods (Backward Stepwise)

- Start with every term in the model
- Consider all models with one predictor removed
- Remove the term that leads to the biggest score improvement
- Repeat until removing additional terms doesn't improve your model

## Sequential methods

- There are many potential models usually exhausting the model space is difficult or infeasible
- Stepwise methods don't consider all possibilities
- Stepwise methods work well for *F* and *t*-tests, which require nested models
- Other criteria don't require nested models (which can be nice) but don't ascertain significance (which can be a downer)

## Sequential methods

Sequential methods are basically an admission that you had no idea what you were doing with the data



AIC ("An Information Criterion") measures goodness-of-fit through RSS (equivalently, log likelihood) and penalizes model size:

$$AIC = n\log(RSS/n) + 2p$$

- Small AIC's are better, but scores are not directly interpretable
- Penalty on model size tries to induce *parsimony*

BIC ("Bayes Information Criterion") similarly measures goodness-of-fit through RSS (equivalently, log likelihood) and penalizes model size:

$$BIC = n \log(RSS/n) + p \log(n)$$

- Small BIC's are better, but scores are not directly interpretable
- AIC and BIC measure goodness-of-fit through RSS, but use different penalties for model size. They won't always give the same answer

## Adjusted $R^2$

Recall:

$$R^2 = 1 - \frac{RSS}{TSS}$$

Definition of adjusted R<sup>2</sup>:

$$R_a^2 = 1 - \frac{RSS/(n-p-1)}{TSS/(n-1)} = 1 - \frac{\hat{\sigma}_{model}^2}{\hat{\sigma}_{null}^2}$$
$$= 1 - \frac{n-1}{n-p-1}(1-R^2)$$

- Minimizing the standard error of prediction means minimizing 
   <sup>2</sup><sub>model</sub> which in turn means maximizing R<sup>2</sup><sub>a</sub>
- Adding a predictor will not necessarily increase R<sub>a</sub><sup>2</sup> unless it has some predictive value

#### PRESS

Prediction residual sum of squares is the most clearly focused on prediction

$$PRESS = \sum (y_i - \boldsymbol{x}_i^T \hat{\boldsymbol{\beta}}_{(-i)})^2$$

Looks computationally intensive, but for linear regression models this is equivalent to

$$PRESS = \sum \left(\frac{r_i}{1 - h_{ii}}\right)^2$$

PRESS is leave-one-out cross validation; other forms of cross validation are equally vaid

# Life expectancy example

- Response: life expectancy
- Predictors: population, capital income, illiteracy rate, murder rate, percentage of high-school graduates, number of days with minimum temperature < 32, land area</li>
- Data for 50 US states
- Time span: 1970-1975

```
> data(state)
> statedata = data.frame(state.x77,row.names=state.abb)
> g = lm(Life.Exp ~., data=statedata)
> summary(g)
...
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	7.094e+01	1.748e+00	40.586	< 2e-16	* * *
Population	5.180e-05	2.919e-05	1.775	0.0832	
Income	-2.180e-05	2.444e-04	-0.089	0.9293	
Illiteracy	3.382e-02	3.663e-01	0.092	0.9269	
Murder	-3.011e-01	4.662e-02	-6.459	8.68e-08	* * *
HS.Grad	4.893e-02	2.332e-02	2.098	0.0420	*
Frost	-5.735e-03	3.143e-03	-1.825	0.0752	
Area	-7.383e-08	1.668e-06	-0.044	0.9649	

...
> AIC(g)
[1] 121.7092

```
> g = lm(Life.Exp ~ . - Area, data=statedata)
> summary(g)
...
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	7.099e+01	1.387e+00	51.165	< 2e-16	* * *
Population	5.188e-05	2.879e-05	1.802	0.0785	
Income	-2.444e-05	2.343e-04	-0.104	0.9174	
Illiteracy	2.846e-02	3.416e-01	0.083	0.9340	
Murder	-3.018e-01	4.334e-02	-6.963	1.45e-08	* * *
HS.Grad	4.847e-02	2.067e-02	2.345	0.0237	*
Frost	-5.776e-03	2.970e-03	-1.945	0.0584	

...
> AIC(g)
[1] 119.7116

```
> g = lm(Life.Exp ~ . - (Area + Illiteracy), data=statedata)
> summary(g)
...
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	7.107e+01	1.029e+00	69.067	< 2e-16	* * *
Population	5.115e-05	2.709e-05	1.888	0.0657	
Income	-2.477e-05	2.316e-04	-0.107	0.9153	
Murder	-3.000e-01	3.704e-02	-8.099	2.91e-10	* * *
HS.Grad	4.776e-02	1.859e-02	2.569	0.0137	*
Frost	-5.910e-03	2.468e-03	-2.395	0.0210	*

... > AIC(g) [1] 117.7196

```
> g = lm(Life.Exp ~ . - (Area + Illiteracy + Income), data=statedata)
> summary(g)
...
```

Coefficients:

```
        Estimate
        Std. Error t value
        Pr(>|t|)

        (Intercept)
        7.103e+01
        9.529e-01
        74.542
        < 2e-16</td>
        ***

        Population
        5.014e-05
        2.512e-05
        1.996
        0.05201
        .

        Murder
        -3.001e-01
        3.661e-02
        -8.199
        1.77e-10
        ***

        HS.Grad
        4.658e-02
        1.483e-02
        3.142
        0.00297
        **

        Frost
        -5.943e-03
        2.421e-03
        -2.455
        0.01802 *
```

...
> AIC(g)
[1] 115.732

```
> g = lm(Life.Exp ~ . - (Area + Illiteracy + Income + Population), data=statedata)
> summary(g)
...
```

 Coefficients:

 Estimate Std. Error t value Pr(>|t|)

 (Intercept)
 71.036379
 0.983262
 72.246
 < 2e-16</td>
 \*\*\*

 Murder
 -0.283065
 0.036731
 -7.706
 8.04e-10
 \*\*\*

 HS.Grad
 0.049949
 0.015201
 3.286
 0.00195
 \*\*

 Frost
 -0.006912
 0.002447
 -2.824
 0.00699 \*\*

...
> AIC(g)
[1] 117.9743

#### So now what?

- It's common to treat the final model as if it were the only model ever considered – to base all interpretation on this model and to assume the inference is accurate
- This doesn't really reflect the true model building procedure, and can misrepresent what actually happened
- Inference is difficult in this case; it's hard to write down a statistical framework for the entire procedure
- Predictions can be made from the final model, but uncertainty around predictions will be understated
- P-values, CIs, etc will be incorrect

### What to do?

- Remember the bootstrap?
- We can resample subjects with replacement, and repeat the entire process
- Produce predicted values  $\hat{y}_i^b$  for  $x = \{x_i\}_{i=1}^I$  based on the final bootstrap model
- Base inference for predictions on the distribution of  $\{\hat{y}_i^b\}_{b=1}^B$

Downside – only gives inference for predicted values, not for the parameter estimates. Bootstrap models might not be the same as the final model (which is kind of the point).

# Shrinkage/penalization

As a preview of things to come -

- There are other strategies for model/variable selection or tuning
- *Penalized regression* adds an explicit penalty to the least squares criterion
- That penalty can keep regression coefficients from being too large, or can shrink coefficients to zero
- We'll worry more about this next time

## Variable selection in polynomial models

A quick note about polynomials. If you fit a model of the form

$$y_i = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon_i$$

and find the quadratic term is significant but the linear term is not...

- You should still keep the linear term in the model
- Otherwise, your model is sensitive to centering shifting x will change your model

### Today's big ideas

Model selection

Suggested reading: Ch 10