Data, Environment and Society: Lecture 10: Multiple Regression

Instructor: Duncan Callaway
GSI: Salma Elmallah

October 1, 2019

Today

- First: Finish reviewing Jupyter notebook on confidence intervals.
  - Objective: understand how a distribution of parameter values is possible when you train OLS with a sample from a population.
- Next: slides, covering multiple regression and (one form of) model selection. Slides in GitHub
  - Model selection is the method for dealing with bias-variance tradeoff
  - It is one of the most important processes we do in statistical learning
- Third: Introduction to land use regression, start working with NO2 data in Jupyter notebook
  - We'll begin learning about a paper that uses one form of model selection.
  - Later in the semester you'll use the tools from this class to improve on this paper.

Announcements

Reading

- Today: ISLR 3.2
- Thursday: ISLR Ch 3.3.
- Next Tuesday: Novotny *et al*, see questions in GitHub folder for lecture 12 reading.

Survey posted! Please respond

Final project – team and initial idea due Thursday

- You can work with your own data
- But we have also suggested data sets
- Working in groups up to three ok (you can self-organize)
- We will give you basic guardrails on what to do
  - Pose a coherent question that can be addressed using the skills we are learning
  - EDA and visualization requirements
  - Carry out multiple prediction exercises using the tools we are learning.
  - Critique the performance of your models
  - Interpret your results within the confines of what your models are capable of.

What if the confidence interval contains zero?

For example, if

$$-10.3 < \beta_1 < 24.8?$$

...where the upper and lower bounds comprise the 95% confidence interval.

What if the confidence interval contains zero?

For example, if

$$-10.3 < \beta_1 < 24.8?$$

...where the upper and lower bounds comprise the 95% confidence interval.

This implies there is more than a remote chance that there is no significant relationship between the dependent and independent variables.

p-values

What are they?

p-values

What are they? p-values measure the probability that the estimated coefficients arose by chance from a data generating process that actually has *no* relationship between the inputs and outputs.

$p = 0.05$ implies a 5% chance that the true parameter value is *zero*.

If $p \ll 0.05$, then the parameter is strongly inside the 95% confidence interval.

If $p > 0.05$, then the parameter is outside the 95% confidence interval.

A small p-value indicates that it is unlikely to observe such a substantial association between the predictor and the response due to chance.

p-hacking?

What's wrong with these practices:

- Stop collecting data once $p < 0.05$
- Analyze many independent variables, but only report those for which $p < 0.05$
- Collect and analyze many data samples, but only report those with $p < 0.05$
- Exclude participants to get $p < 0.05$.
- Transform the data to get $p < 0.05$.

(credit to Leif Nelson, UCB Haas)

The trouble with p-hacking...

...is that by looking for the data set and the models that give low p-values, you could just be looking for those 5% “chances” where the real relationship is non-existent.

In other words, if you flip a coin with 5% probability it’ll turn up heads enough times, eventually you get heads.

In the case of p-hacking, a getting a p-value of 5% when there really is no relationship is the analogy to getting heads on that 5% probability coin.

The trouble with p-hacking...

...is that by looking for the data set and the models that give low p-values, you could just be looking for those 5% “chances” where the real relationship is non-existent.

In other words, if you flip a coin with 5% probability it’ll turn up heads enough times, eventually you get heads.

In the case of p-hacking, a getting a p-value of 5% when there really is no relationship is the analogy to getting heads on that 5% probability coin.

Some estimates suggest that this practice leads to false positive rates of 61%!

The origins of p-hacking

Why do people do it?

The origins of p-hacking

Why do people do it?

One explanation: Researchers are deliberately deceiving their peers. They want good results so they go fisihing for them.

The origins of p-hacking

Why do people do it?

One explanation: Researchers are deliberately deceiving their peers. They want good results so they go fisihing for them.

Maybe, but...

- perhaps people simply don't understand the idea that their parameters are one draw from a *distribution* of possible parameters
- and therefore they don't really understand how to interpret p.

Now you understand – so my hope is that you'll always interpret these with caution!

Model accuracy: R^2

TSS = total sum of squares

RSS = residual sum of squares

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

Model accuracy: R^2

TSS = total sum of squares

RSS = residual sum of squares

$$R^2 = \frac{TSS - RSS}{TSS} = \frac{\sum_{i=1}^{n}(y_i - \bar{y})^2 - \sum_{i=1}^{n} e_i^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

Model accuracy: R^2

TSS = total sum of squares

RSS = residual sum of squares

$$R^2 = \frac{TSS - RSS}{TSS} = \frac{\sum_{i=1}^{n}(y_i - \bar{y})^2 - \sum_{i=1}^{n} e_i^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} = 1 - \frac{\sum_{i=1}^{n} e_i^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

R^2 measures the fraction of variation in the dependent variable that is captured by the model.

Model accuracy: R^2

TSS = total sum of squares

RSS = residual sum of squares

$$R^2 = \frac{TSS - RSS}{TSS} = \frac{\sum_{i=1}^{n}(y_i - \bar{y})^2 - \sum_{i=1}^{n} e_i^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} = 1 - \frac{\sum_{i=1}^{n} e_i^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

R^2 measures the fraction of variation in the dependent variable that is captured by the model.

It's good for capturing predictive power, but not for evaluating the significance of the model.

Let's be clear...

What do people doing prediction care about, $\hat{\beta}$ or $\hat{y}$?

Let's be clear...

What do people doing prediction care about, $\hat{\beta}$ or $\hat{y}$?

$\hat{y}$!

Let's be clear...

What do people doing prediction care about, $\hat{\beta}$ or $\hat{y}$?

$\hat{y}$!

What measure should people doing prediction use to evaluate model performance, coefficient confidence intervals, RSS, R^2 or p?

Let's be clear...

What do people doing prediction care about, $\hat{\beta}$ or $\hat{y}$?

$\hat{y}$!

What measure should people doing prediction use to evaluate model performance, coefficient confidence intervals, RSS, R^2 or p?

RSS or R^2 are suitable. But there is much more to the story!

- Today we'll talk about adjustments to R^2 that attempt to address bias-variance tradeoff
- We'll discuss other approaches in the coming weeks.

Multivariate regression

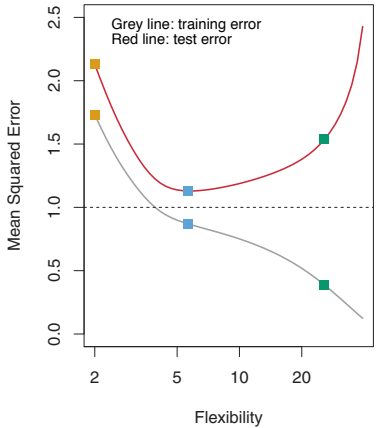
This is exactly the same process as single (independent) variable regression: minimize mean squared error (MSE). Parameter solutions can be found by

- Gradient search
- Normal equations
- Setting partial derivatives of MSE to zero and solving – but now for $\beta_0, \beta_1, \beta_2, \ldots, \beta_d$ (d is the number of features, a.k.a. independent variables).

The mechanics of finding parameters is easy. The real challenge is: Which features to include?

Model selection

The challenge: Don't include variables in your model that lead to over-fit.



With multiple regression, increasing the number of variables increases the flexibility of the model.

Model selection methods

Two basic methods:

- Computationally heavy and theoretically robust:
  - repeated sampling of train and test data sets
  - build and test models with each sampled set
  - choose the model form that minimizes test error, on average.
  - the figure on the previous slide is an example of this approach.

- Easy to implement (no need for significant computing):
  - Use the full data set
  - Fit each candidate model once
  - Choose the model that minimizes an “adjusted” measure of R2 or mean squared error.

An easy-to-implement method

Akaike information criterion (AIC):

1. Construct all the models you have time for using *all* the data (i.e. all your observations) to train the models.
2. Then, choose the model with the lowest AIC, where

$$\text{AIC} = \frac{1}{n\hat{\sigma}^2}(\text{RSS} + 2d\hat{\sigma}^2)$$

$\hat{\sigma}$ is an estimate of the variance of the error ϵ.

An easy-to-implement method

Akaike information criterion (AIC):

1. Construct all the models you have time for using *all* the data (i.e. all your observations) to train the models.
2. Then, choose the model with the lowest AIC, where

$$\text{AIC} = \frac{1}{n\hat{\sigma}^2}(\text{RSS} + 2d\hat{\sigma}^2) = \frac{1}{\hat{\sigma}^2}\left(\frac{\text{RSS}}{n}\right) + \frac{2d}{n}$$

$\hat{\sigma}$ is an estimate of the variance of the error ϵ.

As you can see, AIC "penalizes" models with a high value of d.

What the heck is AIC?

It actually has a rigorous theoretical underpinning. Understanding the derivation requires background in information theory and more time than we have here.

What the heck is AIC?

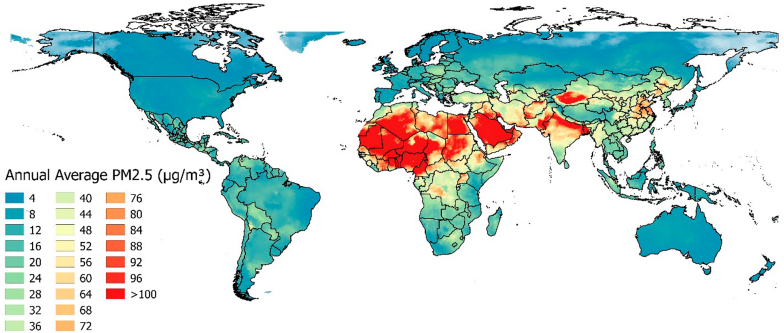
It actually has a rigorous theoretical underpinning. Understanding the derivation requires background in information theory and more time than we have here.

But:

- It gives unbiased estimate of the MSE you'd get if you *did* use a test data set (as long as the errors are Gaussian)
- It's ok to just work with the intuition that choosing models that minimize AIC is analogous to
  - choosing models that minimize MSE ...
  - plus a penalty for the number of features.

Prediction application: Land use regression

- Suppose we'd like to know pollutant concentrations at a fine spatial resolution
- We only have pollutant measurements at low resolution (coarse spatial scale)
- But we have other measurements at finer spatial resolution
- This is an ideal job for forecasting.
- But rather than forecast in *time* we will forecast in *space*.



(From Shaddick *et al* ES&T 2018)

Nitrogen dioxide

NO_2:

- Direct product of fossil fuel combustion
- Used as an indicator for larger group of nitrogen oxides.
- Health impact: Contributes to development of, and aggravates, asthma
- Environmental impact: Haze, acid rain, nutrient pollution in coastal waters

EPA Regulates NO2:

Nitrogen Dioxide (NO_2)	primary	1 hour	100 ppb	98th percentile of 1-hour daily maximum concentrations, averaged over 3 years
	primary and secondary	1 year	53 ppb [(2)]	Annual Mean

(Primary standards are designed to protect public health. Secondary standards are designed to address visibility, crop protection, damage to buildings, and so on.)

Novotny *et al* setup

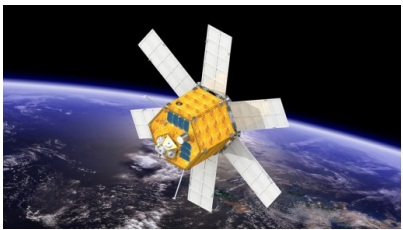
- NO_2 concentrations are known where monitors are present.
- But we don't have monitors everywhere
- Can we *predict* concentrations where monitors are absent?

Novotny *et al* setup

- NO_2 concentrations are known where monitors are present.
- But we don't have monitors everywhere
- Can we *predict* concentrations where monitors are absent?

"Remote sensing" data from satellites can be useful:

- Aurora satellite "Ozone Monitoring Instrument" provides tropospheric NO2 column abundance (units: ppb; Called "WRF+DOMINO" in data set we'll work with).



Novotny *et al* setup

- NO_2 concentrations are known where monitors are present.
- But we don't have monitors everywhere
- Can we *predict* concentrations where monitors are absent?

"Remote sensing" data from satellites can be useful:

- Aurora satellite "Ozone Monitoring Instrument" provides tropospheric NO2 column abundance (units: ppb; Called "WRF+DOMINO" in data set we'll work with).

But!

- Measurements are for entire column of air above a location, not ground-level
- Spatial resolution is low

Land use regression for NO_2

Dependent variable: Hourly NO_2 concentrations from EPA sensors.

Independent variables to consider:

parameter	units	spatial resolution	buffer[a] or point estimate
impervious surface	%	30 m (United States only[32]); 1000 m (global[29])	buffer
tree canopy	%	30 m (United States only[33]); 500 m (global[30])	buffer
population	no.	Census block (United States only[34]); 1 km (global[31])	buffer
major road length[35]	km	NA	buffer
minor road length[35]	km	NA	buffer
total road length[35]	km	NA	buffer
elevation[36]	km	90 m	point
distance to coast	km	NA	point
OMI NO_2[25,26]	ppb	13×24 km^2 at nadir	point

Novotny *et al* Table 1.

Let's run some linear regression models with these data. Move over to Jupyter notebook for today's lecture.