Data, Environment and Society: Lecture 10: Multiple Regression

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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?

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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?

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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.

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

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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 $= \sum_{i=1}^{n} (y_i - \bar{y})^2$

RSS = residual sum of squares $\sum_{i=1}^{n} (y_i - \hat{y}_i)^2$

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

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

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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

$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{1i} + \hat{\beta}_2 X_{2i}$

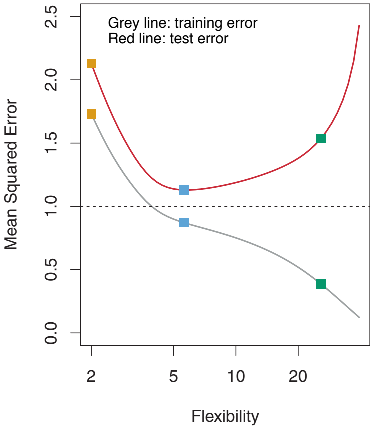
This is exactly the same process as single (independent) variable regression: minimize mean squared error (MSE). Parameter solutions can be found by

- 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

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

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

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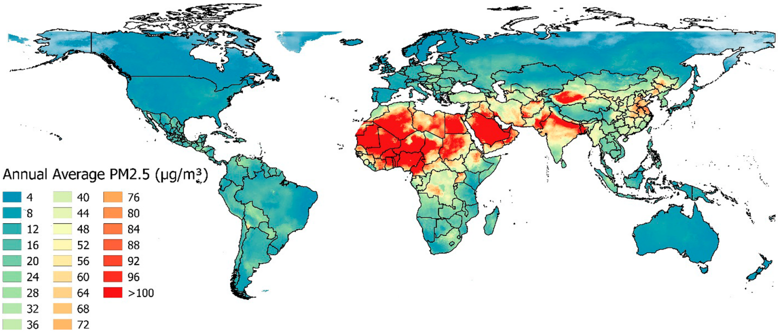
But:

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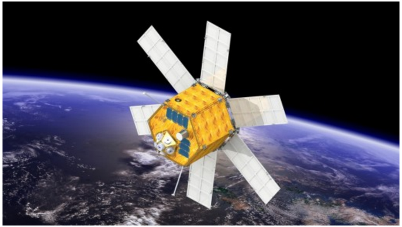
- Aurora satellite "Ozone Monitoring Instrument" provides tropospheric NO2 column abundance (units: ppb; Called "WRF+DOMINO" in data set we'll work with).



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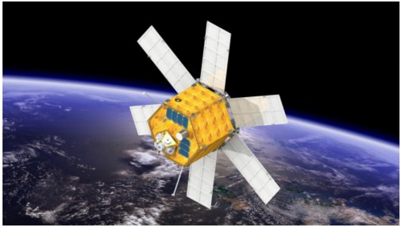

But!

- 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.