Lecture 3: OLS & Prediction in/out of Sample

Big Data and Machine Learning for Applied Economics
Econ 4676

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Agenda

Recap

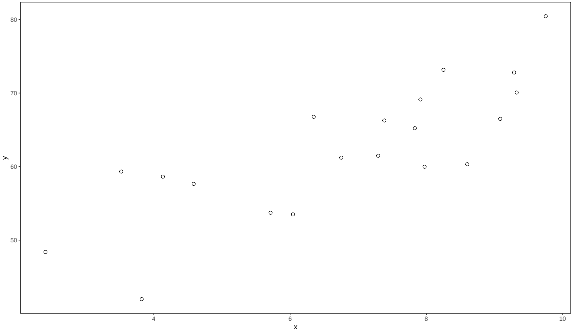
- We started shifting paradigms
- Decision Theory: Risk with square error loss $\rightarrow$ MSE
- Objective minimize the reducible error
- Irreducible error our unknown bound
- Machine Learning best kept secret: some bias can help lower MSE

Motivation

- Linear regression is the “work horse” of econometrics and (supervised) machine learning.
- Very powerful in many contexts:
  - Model Spatial Relationships
  - Non linear relationships
- It can be used also for classification.
- Big ‘payday’ to study this model in detail.

Linear Regression Model

Problem



Linear Regression Model

$f(X) = X\beta$ and the interest is on estimating β

$$y = X\beta + u \tag{1}$$

where

- y is a vector $n \times 1$ with typical element y_i
- X is a matrix $n \times k$
  - Note that we can represent it as a column vector $\underset{n\times k}{X} = [\underset{n\times 1}{X_1} \; \underset{n\times 1}{X_2} \; \dots \; \underset{n\times 1}{X_k}]$
- β is a vector $k \times 1$ with typical element β_j

Thus

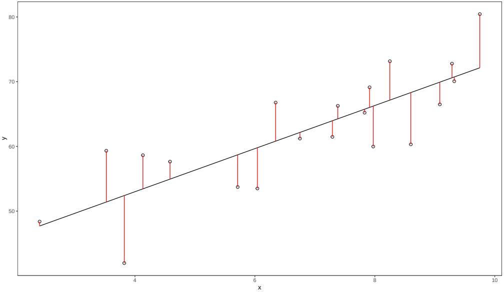
$$\begin{aligned} y_i &= X_i'\beta + u_i \\ &= \sum_{k=1}^{k} \beta_j X_{ji} + u_i \end{aligned} \tag{2}$$

Linear Regression Model

How do we estimate β?

- Method of Moments (for HW)
- MLE (more on this later)
- OLS: minimize risk squared error loss $\rightarrow$ minimizes RSS ($e'e$)
  - where $e = Y - \hat{Y} = Y - X\hat{\beta}$
  - In the HW, you will show that min RSS same as max R^2

OLS solution: $\hat{\beta} = (X'X)^{-1}X'y$



Gauss Markov Theorem

Gauss-Markov Theorem says that

$$\hat{\beta} = (X'X)^{-1}X'y \tag{3}$$

- The OLS estimator ($\hat{\beta}$) is BLUE, the more efficient than any other linear unbiased estimator,
- Efficiency in the sense that $Var(\tilde{\beta}) - Var(\hat{\beta})$ is positive semidefinite matrix.

Proof: HW. Tip: a matrix $M_{p\times p}$ is positive semi-definite iff $c'Mc \geq 0 \; \forall x \in \mathbb{R}^p$

Gauss Markov Theorem

- Gauss Markov Theorem that says OLS is BLUE is perhaps one of the most famous results in statistics.
  - $E(\hat{\beta}) = \beta$
  - $V(\hat{\beta}) = \sigma^2 (X'X)^{-1}$
- However, it is essential to note the limitations of the theorem.
  - Correctly specified with exogenous Xs,
  - The term error is homoscedastic
  - No serial correlation.
  - Nothing about the OLS estimator being the more efficient than any other estimator one can imagine.

Prediction vs Estimation

- **Predicting well means estimating well**
  - Note that the prediction of y will be given by $\hat{y} = X\hat{\beta}$
  - Under Gauss-Markov framework
    - $E(\hat{y}) = X\beta$
    - $V(\hat{y}) = \sigma^2 X'(X'X)^{-1}X$
- Then if $\hat{\beta}$ is unbiased and of minimum variance,
- then $\hat{y}$ is an unbiased predictor and minimum variance, from the class of unbiased linear estimators/predictors
  - Proof: for HW similar to $\hat{\beta}$ proof

Prediction vs Estimation

- **Estimation Accuracy**

$$MSE(\beta) = E(\hat{\beta} - \beta) \tag{4}$$

$$= E(\beta - E(\hat{\beta}))^2 + Var(\hat{\beta}) \tag{5}$$

- Intuitively, the result says that how wrong is the estimate (MSE) depends on:
  - how uncentered it is (bias) and
  - how dispersed it is around its center (variance).

Prediction and Predictive Error

- Now suppose that the goal is to predict Y with another random variable $\hat{Y}$.
- The *prediction error* is defined as:

$$Err(\hat{Y}) \equiv E\left(Y - \hat{Y}\right)^2 \tag{6}$$

- Conceptually the prediction error is equal to the MSE
- However, MSE compares a RV ($\hat{\beta}$) with a parameter (β)
- $Err(\hat{Y})$ involves two RV

Prediction and predictive error

- More concretely, the goal is to predict Y given another variable X.
- We assume that the link between Y and X is given by the simple model:

$$Y = f(X) + u \tag{7}$$

- where $f(X)$ is any function,
- u is an unobserved random variable with $E(u) = 0$ and $V(u) = \sigma^2$

Prediction and predictive error

- In practice we don't observe $f(X)$
- We need to estimate it with $\hat{f}(X)$ a RV

Then

$$Err(\hat{Y}) = MSE(\hat{f}) + \sigma^2 \tag{8}$$
$$= Bias^2(\hat{f}) + V(\hat{f}) + \sigma^2 \tag{9}$$

Two parts:

- the error from estimating f with $\hat{f}$. (*reducible*)
- the error from not being able to observe u. (*irreducible*)

This is an important result, predicting Y properly we need a good estimate of f.

Prediction and Linear regression

- Linear regression sets

$$f(X) = \beta_1 + \beta_2 X_2 + \cdots + \beta_k X_k \tag{10}$$

- In classical econometrics this model is given
- Focus is on the estimation of the unknown parameters $\beta_1, \ldots, \beta_k$.
- The prediction for Y is given by:

$$\hat{Y} = \hat{\beta}_1 + \hat{\beta}_2 X_2 + \cdots + \hat{\beta}_k X_k \tag{11}$$

- where $\hat{\beta}_1, \ldots, \hat{\beta}_k$ are estimates.

Prediction and linear regression

- Under the classical assumptions the OLS estimator is unbiased, hence

$$
\begin{aligned}
E(\hat{f}) &= E(\hat{\beta}_1 + \hat{\beta}_2 X_2 + \cdots + \hat{\beta}_k X_k) && (12)\\
&= E(\hat{\beta}_1) + E(\hat{\beta}_2) X_2 + \cdots + E(\hat{\beta}_k) X_k && (13)\\
&= f && (14)
\end{aligned}
$$

Then,

- $MSE(\hat{f})$ reduces to just $V(\hat{f})$

Complexity and the variance/bias trade off

- When the focus switches from estimating f to predicting Y,
- f plays a secondary role, as just a tool to improve the prediction based on X.
- Predicting Y involves *learning* f, that is, f is no longer taken as given, as in the classical view.
- Now it implies an iterative process where initial choices for f are revised in light of potential improvements in predictive performance.
- Model choice or learning involves choosing both f and a strategy to estimate it ($\hat{f}$), guided by predictive performance.

Complexity and the variance/bias trade off

- Classical econometrics, model choice involves deciding between a smaller and a larger linear model.
- Consider the following competing models for y:

$$Y = \beta_1 X_1 + u_1 \tag{15}$$

and

$$Y = \beta_1 X_1 + \beta_2 X_2 + u_2 \tag{16}$$

- $\hat{\beta}_1^{(1)}$ the OLS estimator of regressing y on X_1
- $\hat{\beta}_1^{(2)}$ and $\hat{\beta}_2^{(2)}$ the OLS estimators of β_1 and β_2 of regressing Y on X_1 and X_2.

Complexity and the variance/bias trade off

The corresponding predictions will be

$$\hat{Y}^{(1)} = \hat{\beta}_1^{(1)} X_1 \tag{17}$$

and

$$\hat{Y}^{(2)} = \hat{\beta}_1^{(2)} X_1 + \hat{\beta}_2^{(2)} X_2 \tag{18}$$

Complexity and the variance/bias trade off

- An important discussion in classical econometrics is that of omission of relevant variables vs. inclusion of irrelevant ones.
  - If model (1) is true then estimating the larger model (2) leads to inefficient though unbiased estimators due to unnecessarily including X_2.
  - If model (2) holds, estimating the smaller model (1) leads to a more efficient but biased estimate if X_1 is also correlated with the omitted regressor X_2.

- this discussion of small vs large is always with respect to a model that is supposed to be true.

- But in practice the true model is unknown.

Complexity and the variance/bias trade off

- Choosing between models involves a *bias/variance trade off*
- Classical econometrics tends to solve this dilemma abruptly,
  - requiring unbiased estimation, and hence favoring larger models to avoid bias
- In this simple setup, larger models are 'more complex', hence more complex models are less biased but more inefficient.
- Hence, in this very simple framework complexity is measured by the number of explanatory variables.
- A central idea in machine learning is to generalize the idea of complexity,
  - Optimal level of complexity, that is, models whose bias and variance led to minimum MSE.

Train and Test Samples

- A goal of machine learning is *out of sample* prediction
- OLS estimator minimizes the sum of squared residuals and hence maximizes R^2 through maximizing the explained sum of squares.
- OLS is designed to optimize the predictive power of the model, for the data used for estimation.
- But in most predictive situations what really matters is the ability to predict new data.

Train and test samples

- A simple alternative would be to split the data into two groups
  - Training sample: to build/estimate/train the model
  - Test sample: to evaluate its performance
- From a strictly classical perspective
  - Makes sense if training data is iid from the population, even works if it is iid conditional on X
  - Two problems with this idea:
    - The first one is that given an original data set, if part of it is left aside to test the model, less data is left for estimation.
    - A second problem is how to decide which data will be used to train the model and which one to test it. (more on how cross validation helps later)

Train and test samples

The *estimated prediction error* is defined as

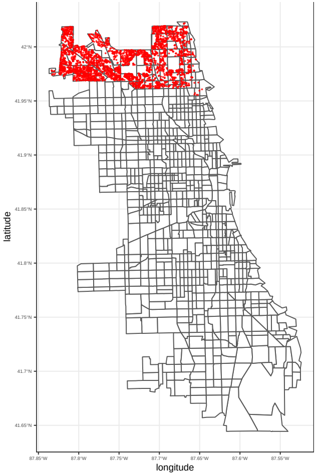
$$\hat{Err}(\hat{Y}) = \sum_{i \in Test\ Sample} \left(Y_i - \hat{Y}_i\right)^2 \tag{19}$$

- $i \in Test\ Sample$ refers to all the observations in the test sample.
- $Test\ Sample \cup Training\ Sample = \ Full\ Sample$
- Note that:
  - No obvious way on how to partition this
  - In some cases is exogenously given. `Kaggle Competition`, `Netflix Challenge`
  - This idea is almost inexistent (or trivial) in classical econometrics

Example: Predicting House Prices in R

- `matchdata` in the *McSpatial package* for R.
- 3,204 sales of SFH Far North Side of Chicago in 1995 and 2005.
- This data set includes 18 variables/features about the home,
  - price sold
  - number of bathrooms, bedrooms,
  - latitude and longitude,
  - etc.
- in R:

```
require(mcmspatial)#loads the package
data(matchdata) #loads the data
?matchdata # help/info about the data
```



Example: Predicting House Prices in R

- Train and Test samples
- 70% / 30% split

```
set.seed(101010) #sets a seed
matchdata <- matchdata %>%
                      mutate(price=exp(lnprice),
                             #transforms log prices to standard prices
                             holdout= as.logical(1:nrow(matchdata)
                             %in% sample(
                             nrow(matchdata), nrow(matchdata)*.7))
                             #generates a logical indicator
                             )

test<-matchdata[matchdata$holdout==T,]
train<-matchdata[matchdata$holdout==F,]
```

Example: Predicting House Prices in R

- Naive approach: model with no covariates, just a constant
- $y = \beta_0 + u$

```
model1<-lm(price~1,data=train)
summary(model1)
```

```
##
## Call:
## lm(formula = price ~ 1, data = train)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -258018 -127093  -24018   92732  598482
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   284018       4782   59.39   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 148300 on 961 degrees of freedom
```

Example: Predicting House Prices in R

In this case our prediction for the log price is the average train sample average

$$\hat{y} = \hat{\beta}_0 = \frac{\sum y_i}{n} = m$$

```
coef(model1)
```

```
## (Intercept)
##    284017.6
```

```
mean(train$price)
```

```
## [1] 284017.6
```

Example: Predicting House Prices in R

- But we are concerned on predicting well our of sample,:

```
test$model1<-predict(model1,newdata = test)
with(test,mean((price-model1)^2))
```

```
## [1] 21935777917
```

- $\hat{A}Err(\hat{y}) = \frac{\sum((y-\hat{y})^2)}{n} = 2.1935778 \times 10^{10}$
- This is our starting point, Can we improve it?

Example: Predicting House Prices in R

- How to improve it?
  - One way is using econ theory as guide
  - hedonic house price function derived directly from the Rosen's theory of hedonic pricing
  - however, the theory says little on what are the relevant attributes of the house.
  - So we are going to explore the effects of adding house characteristics on our out $AErr(\hat{y})$
- The simple inclusion of a single covariate can improve with respect to the *naive* constant only model.

```
model2<-lm(price~bedrooms,data=train)
test$model2<-predict(model2,newdata = test)
with(test,mean((price-model2)^2))
```

```
## [1] 21695551442
```

Example: Predicting House Prices in R

- What about if we include more variables?

```
model3<-lm(price~bedrooms+bathrooms+centair+fireplace+brick,data=train)
test$model3<-predict(model3,newdata = test)
with(test,mean((price-model3)^2))
```

```
## [1] 21111169595
```

- Note that the *AErr* is once more reduced. If we include all?

```
model4<-lm(price~bedrooms+bathrooms+centair+fireplace+brick+
                lnland+lnbldg+rooms+garage1+garage2+dcbd+rr+
                yrbuilt+factor(carea)+latitude+longitude,data=train)
test$model4<-predict(model4,newdata = test)
with(test,mean((price-model4)^2))
```

```
## [1] 20191829518
```

- Is there a limit to this improvement? Can we keep adding features and complexity?

Example: Predicting House Prices in R

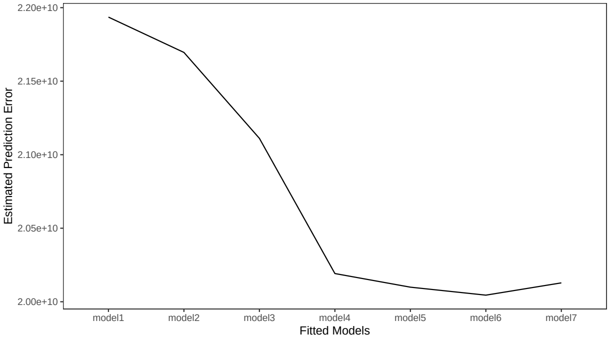
- Is there a limit to this improvement? Can we keep adding features and complexity?
- Let's try a bunch of models

```
model5<-lm(price~poly(bedrooms,2)+poly(bathrooms,2)+
                centair+fireplace+brick+
                lnland+lnbldg+rooms+
                garage1+garage2+dcbd+rr+
                yrbuilt+factor(carea)+poly(latitude,2)+
                poly(longitude,2),data=train)
test$model5<-predict(model5,newdata = test)

model6<-lm(price~poly(bedrooms,2)+poly(bathrooms,2)+centair+fireplace+brick+
                lnland+lnbldg+garage1+garage2+rr+
                yrbuilt+factor(carea)+poly(latitude,2)+poly(longitude,2),
                data=train)
test$model6<-predict(model6,newdata = test)

model7<-lm(price~poly(bedrooms,2)+poly(bathrooms,2)+centair+fireplace+brick+
                lnland+lnbldg+garage1+garage2+rr+
                yrbuilt+factor(carea)+poly(latitude,3)+poly(longitude,3),
                data=train)
test$model7<-predict(model7,newdata = test)
```

Example: Predicting House Prices in R



- Take aways from the example
- Classical econometrics set up, choosing between smaller and larger models
- More complexity, the prediction error keeps getting smaller.
- The choice of a model's complexity faces a bias/variance trade-off.
- Open question: how to find the optimal complexity level?

  (later on the course)

Review & Next Steps

- Linear Regression
- Prediction vs Estimation
- Train and Test Samples
- Example in R

- **Next Class:** Big Data intro, OLS Numerical Properties Computation.

- Questions? Questions about software?

Further Readings

- Davidson, R., & MacKinnon, J. G. (2004). Econometric theory and methods (Vol. 5). New York: Oxford University Press.
- James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). An introduction to statistical learning (Vol. 112, p. 18). New York: springer.
- Friedman, J., Hastie, T., & Tibshirani, R. (2001). The elements of statistical learning (Vol. 1, No. 10). New York: Springer series in statistics.
- Murphy, K. P. (2012). Machine learning: a probabilistic perspective. MIT press.