

STAT151A Homework 6: Due April 19th

Your name here

1 Fit and regressors

Given a regression on \mathbf{X} with P regressors, and the corresponding \mathbf{Y} , $\hat{\mathbf{Y}}$, and $\hat{\varepsilon}$, define the following quantities:

$$RSS := \hat{\varepsilon}^\top \hat{\varepsilon} \quad (\text{Residual sum of squares})$$

$$TSS := \mathbf{Y}^\top \mathbf{Y} \quad (\text{Total sum of squares})$$

$$ESS := \hat{\mathbf{Y}}^\top \hat{\mathbf{Y}} \quad (\text{Explained sum of squares})$$

$$R^2 := \frac{ESS}{TSS}.$$

a

1. Prove that $RSS + ESS = TSS$.
2. Express R^2 in terms of TSS and RSS .
3. What is R^2 when we include no regressors? ($P = 0$)
4. What is R^2 when we include N linearly independent regressors? ($P = N$)
5. Can R^2 ever decrease when we add a regressor? If so, how?
6. Can R^2 ever stay the same when we add a regressor? If so, how?
7. Can R^2 ever increase when we add a regressor? If so, how?
8. Does a high R^2 mean the regression is correctly specified? Why or why not?
9. Does a low R^2 mean the regression is incorrectly specified? Why or why not?

Solutions:

1. This follows from $\hat{\mathbf{Y}}^\top \hat{\varepsilon} = \mathbf{0}$.
2. $R^2 = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$
3. $R^2 = 0$ when we include no regressors
4. $R^2 = 1$ when we include N linearly independent regressors?

5. No, it cannot, since you project onto the same or larger subspace.
6. Yes, if you add a regressor column that is colinear with the existing columns.
7. Yes, if you add a linearly independent regressor column.
8. No, you might overfit.
9. No, you might have low signal to noise ratio.

b

The next questions will be about the F-test statistic for the null $H_0 : \beta = \mathbf{0}$,

$$\phi = \hat{\beta}^\top (\mathbf{X}^\top \mathbf{X}) \hat{\beta} / (P \hat{\sigma}^2)$$

1. Write the F-test statistic ϕ in terms of TSS and RSS , and P .
2. Can ϕ ever decrease when we add a regressor? If so, how?
3. Can ϕ ever stay the same when we add a regressor? If so, how?
4. Can ϕ ever increase when we add a regressor? If so, how?

Solutions:

1. $\phi = \frac{\hat{\mathbf{Y}}^\top \hat{\mathbf{Y}}}{P \text{RSS}/(N-P)} = \frac{N-P}{P} \frac{TSS}{RSS}$
2. Yes, $(N-P)/P$ decreases with P , and TSS and RSS can stay the same if the added regressor is colinear.
3. Yes, TSS/RSS might increase just as much as $(N-P)/P$ decreases.
4. Yes, TSS/RSS might increase more than $(N-P)/P$ decreases.

2 Omitted variable bias

For this problem, let $(\mathbf{x}_n, \mathbf{z}_n, y_n)$ be IID random variables, where $\mathbf{x}_n \in \mathbb{R}^{P_X}$ and $\mathbf{z}_n \in \mathbb{R}^{P_Z}$. Suppose that \mathbf{x}_n and \mathbf{z}_n satisfy $\mathbb{E}[\mathbf{x}_n \mathbf{z}_n^\top] = \mathbf{0}$.

Let $y_n = \mathbf{x}_n^\top \beta + \mathbf{z}_n^\top \gamma + \varepsilon_n$, where ε_n is mean zero, unit variance, and independent of \mathbf{x}_n and \mathbf{z}_n .

a

Take $P_X = P_Z = 1$ (i.e. scalar regressors). Show that there exists x_n and z_n such that $\mathbb{E}[x_n z_n] = 0$ but $\mathbb{E}[z_n | x_n] \neq 0$ for some x_n . (A single counterexample will be enough.)

Solution:

An example is $x_n \sim \mathcal{N}(0, 1)$, and $z_n = x_n^2$. Then $\mathbb{E}[x_n z_n^2] = \mathbb{E}[x_n^3] = 0$.

A general construction is to start with a generic \mathbf{z}_n and define

$$\tilde{\mathbf{z}}_n = \mathbf{z}_n - \mathbb{E}[\mathbf{z}_n \mathbf{x}_n^\top] (\mathbb{E}[\mathbf{x}_n \mathbf{x}_n^\top])^{-1} \mathbf{x}_n.$$

Then

$$\mathbb{E}[\tilde{\mathbf{z}}_n \mathbf{x}_n^\top] = \mathbb{E}[\mathbf{z}_n \mathbf{x}_n^\top] - \mathbb{E}[\mathbf{z}_n \mathbf{x}_n^\top] (\mathbb{E}[\mathbf{x}_n \mathbf{x}_n^\top])^{-1} \mathbb{E}[\mathbf{x}_n \mathbf{x}_n^\top] = \mathbf{0},$$

but

$$\mathbb{E}[\tilde{\mathbf{z}}_n | \mathbf{x}_n^\top] \neq \mathbf{0}$$

if $\mathbb{E}[\mathbf{z}_n | \mathbf{x}_n^\top]$ is not linear in \mathbf{x}_n . So if we start with $\mathbf{z}_n = f(\mathbf{x}_n)$ for any nonlinear function $f(\cdot)$, we get a valid example.

b

Now return to the general case. Let $\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y}$ denote the OLS estimator from the regression on \mathbf{X} alone.

For simplicity, assume that $\frac{1}{N} \sum_{n=1}^N \mathbf{x}_n \mathbf{z}_n^\top = \mathbf{0}$. (Note that, by the LLN, $\frac{1}{N} \sum_{n=1}^N \mathbf{x}_n \mathbf{z}_n^\top \rightarrow \mathbf{0}$ as $N \rightarrow \infty$, so this is a reasonable approximate assumption.)

Derive an expression for $\mathbb{E}[\hat{\beta}]$, where the expectation is taken over \mathbf{X} , \mathbf{Y} , and \mathbf{Z} .

Solution:

$$\begin{aligned} \hat{\beta} &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top (\mathbf{X} \beta + \mathbf{Z} \gamma + \boldsymbol{\varepsilon}) \\ &= \beta + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Z} \gamma + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\varepsilon} \\ &= \beta + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\varepsilon} \Rightarrow \\ \mathbb{E}[\hat{\beta}] &= \beta \end{aligned}$$

c

Using (b), derive an expression for the bias for a fixed \mathbf{x}_{new} , i.e.

$$\mathbb{E}[y_{\text{new}} - \mathbf{x}_{\text{new}}^\top \hat{\beta} | \mathbf{x}_{\text{new}}],$$

in terms of β , γ , and the conditional expectation $\mathbb{E}[\mathbf{z}_{\text{new}} | \mathbf{x}_{\text{new}}]$.

Solution:

$$\begin{aligned}\mathbb{E} \left[y_{\text{new}} - \mathbf{x}_{\text{new}}^T \hat{\beta} | \mathbf{x}_{\text{new}} \right] &= \mathbf{x}_{\text{new}}^T \beta + \mathbb{E} [\mathbf{z}_{\text{new}}^T | \mathbf{x}_{\text{new}}] \gamma + \mathbb{E} [\varepsilon_{\text{new}} | \mathbf{x}_{\text{new}}] - \mathbf{x}_{\text{new}}^T \mathbb{E} [\hat{\beta} | \mathbf{x}_{\text{new}}] \\ &= \mathbb{E} [\mathbf{z}_{\text{new}}^T | \mathbf{x}_{\text{new}}] \gamma.\end{aligned}$$

d

Using your result from (c), show that the predictions are biased at \mathbf{x}_{new} when omitting the variables \mathbf{z}_n from the regression precisely when $\gamma^T \mathbb{E} [\mathbf{z}_n | \mathbf{x}_n] \neq 0$. Using your result from (a), show that this bias can be expected to occur in general — that is, omitting variables can often induce biased predictions at a point.

Solution: This follows directly.

3 Estimating leave-one-out CV

This homework problem derives a closed-form estimate of the leave-one-out cross-validation error for regression. We will use the Sherman-Woodbury formula. Let A denote an invertible matrix, and \mathbf{u} and \mathbf{v} vectors the same length as A . Then

$$(A + \mathbf{u}\mathbf{v}^T)^{-1} = A^{-1} - \frac{A^{-1}\mathbf{u}\mathbf{v}^T A^{-1}}{1 + \mathbf{v}^T A^{-1}\mathbf{u}}.$$

We will also use the following definition of a “leverage score,” $h_n := \mathbf{x}_n^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_n$. We will discuss leverage scores more in the last lecture, but for now it’s enough that you know what it is. Note that $h_n = (\mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T)_{nn}$ is the n -th diagonal entry of the projection matrix \mathbf{P}_X .

Let $\hat{\beta}_{-n}$ denote the estimate of $\hat{\beta}$ with the datapoint n left out. For leave-one-out CV, we want to estimate

$$MSE_{LOO} := \frac{1}{N} \sum_{n=1}^N (y_n - \mathbf{x}_n^T \hat{\beta}_{-n})^2.$$

Note that doing so naively requires computing N different regressions. We will derive a much more efficient formula.

Let \mathbf{X}_{-n} denote the \mathbf{X} matrix with row n left out, and \mathbf{Y}_{-n} denote the \mathbf{Y} matrix with row n left out.

a

Prove that

$$\hat{\beta}_{-n} = (\mathbf{X}_{-n}^\top \mathbf{X}_{-n})^{-1} \mathbf{X}_{-n}^\top \mathbf{Y}_{-n} = (\mathbf{X}^\top \mathbf{X} - \mathbf{x}_n \mathbf{x}_n^\top)^{-1} (\mathbf{X}^\top \mathbf{Y} - \mathbf{x}_n y_n)$$

Solution

This follows from $\mathbf{X}^\top \mathbf{X} = \sum_{n=1}^N \mathbf{x}_n \mathbf{x}_n^\top$ and $\mathbf{X}^\top \mathbf{Y} = \sum_{n=1}^N \mathbf{x}_n y_n$.

b

Using the Sherman-Woodbury formula, derive the following expression:

$$(\mathbf{X}^\top \mathbf{X} - \mathbf{x}_n \mathbf{x}_n^\top)^{-1} = (\mathbf{X}^\top \mathbf{X})^{-1} + \frac{(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \mathbf{x}_n^\top (\mathbf{X}^\top \mathbf{X})^{-1}}{1 - h_n}$$

Solution

Direct application of the formula with $\mathbf{u} = \mathbf{x}_n$ and $\mathbf{v} = -\mathbf{x}_n$ gives

$$(\mathbf{X}^\top \mathbf{X} - \mathbf{x}_n \mathbf{x}_n^\top)^{-1} = (\mathbf{X}^\top \mathbf{X})^{-1} + \frac{(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \mathbf{x}_n^\top (\mathbf{X}^\top \mathbf{X})^{-1}}{1 - \mathbf{x}_n^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n}.$$

Then recognize the leverage score.

c

Combine (a) and (b) to derive the following explicit expression for $\hat{\beta}_{-n}$:

$$\hat{\beta}_{-n} = \hat{\beta} - (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \frac{1}{1 - h_n} \hat{\varepsilon}_n$$

Solution

We have

$$(\mathbf{X}^\top \mathbf{X} - \mathbf{x}_n \mathbf{x}_n^\top)^{-1} \mathbf{X}^\top \mathbf{Y} = \hat{\beta} + \frac{(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \mathbf{x}_n^\top \hat{\beta}}{1 - h_n}.$$

and

$$(\mathbf{X}^\top \mathbf{X} - \mathbf{x}_n \mathbf{x}_n^\top)^{-1} \mathbf{x}_n y_n = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n y_n + \frac{(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n h_n}{1 - h_n} y_n.$$

Combining,

$$\begin{aligned}
\hat{\beta}_{-n} &= \hat{\beta} + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \left(\frac{\mathbf{x}_n^\top \hat{\beta}}{1 - h_n} - y_n - \frac{h_n}{1 - h_n} y_n \right) \\
&= \hat{\beta} + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \left(\frac{1}{1 - h_n} \hat{y}_n - \left(1 + \frac{h_n}{1 - h_n} \right) y_n \right) \\
&= \hat{\beta} + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \left(\frac{1}{1 - h_n} \hat{y}_n - \frac{1}{1 - h_n} y_n \right) \\
&= \hat{\beta} - (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \frac{1}{1 - h_n} \hat{\varepsilon}_n
\end{aligned}$$

d

Using (c), derive the following explicit expression the leave-one-out error on the n -th observation:

$$y_n - \mathbf{x}_n^\top \hat{\beta}_{-n} = \frac{\hat{\varepsilon}_n}{1 - h_n}.$$

Solution

$$\begin{aligned}
y_n - \mathbf{x}_n^\top \hat{\beta}_{-n} &= y_n - \mathbf{x}_n^\top \hat{\beta} + \mathbf{x}_n^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_n \frac{1}{1 - h_n} \hat{\varepsilon}_n \\
&= y_n - \hat{y}_n + \frac{h_n}{1 - h_n} \hat{\varepsilon}_n \\
&= \left(1 + \frac{h_n}{1 - h_n} \right) \hat{\varepsilon}_n \\
&= \frac{\hat{\varepsilon}_n}{1 - h_n}
\end{aligned}$$

e

Using (d), prove that

$$MSE_{LOO} := \frac{1}{N} \sum_{n=1}^N \frac{\hat{\varepsilon}_n^2}{(1 - h_n)^2},$$

where $\hat{\varepsilon}_n = y_n - \hat{y}_n$ is the residual from the full regression without leaving any data out. Using this formula, MSE_{LOO} can be computed using only the original regression and $(\mathbf{X}^\top \mathbf{X})^{-1}$.

Solution Just plug it in.

f

Prove that $\sum_{n=1}^N h_n = P$, and $0 \leq h_n \leq 1$. Hint: if \mathbf{v} is a vector with a 1 in entry n and 0 otherwise, then $h_n = \mathbf{v}^\top \mathbf{P}_X \mathbf{v}$, and projection cannot increase a vector's norm. Recall also that $\text{trace} \left(\mathbf{P}_X \right) = P$.

Solution

$$0 \leq h_n = \mathbf{v}^\top \mathbf{P}_X \mathbf{v} \leq \|\mathbf{v}\|_2^2 = 1,$$

and

$$\sum_{n=1}^N h_n = \text{trace} \left(\mathbf{P}_X \right) = P.$$

g

Using (e) and (f), prove that $MSE_{LOO} > RSS = \frac{1}{N} \sum_{n=1}^N \hat{\varepsilon}_n^2$. That is, the RSS underestimates the leave-one-out cross-validation error.

Solution

We have $1/(1 - h_n)^2 \geq 1$ because $-1 < 0 \leq h_n \leq 1$. At least some $h_n > 0$, since $\sum_{n=1}^N h_n = P$, so for at least one h_n , $1/(1 - h_n)^2 > 1$. The result follows.