STAT151A Homework 6: Due April 19th

Your name here

1 Fit and regressors

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

$$RSS := \hat{\varepsilon}^{\mathsf{T}} \hat{\varepsilon}$$
 (Residual sum of squares)
 $TSS := \mathbf{Y}^{\mathsf{T}} \mathbf{Y}$ (Total sum of squares)
 $ESS := \hat{\mathbf{Y}}^{\mathsf{T}} \hat{\mathbf{Y}}$ (Explained sum of squares)
 $R^2 := \frac{ESS}{TSS}$.

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

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

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

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

2 Omitted variable bias

For this problem, let $(\boldsymbol{x}_n, \boldsymbol{z}_n, y_n)$ be IID random variables, where $\boldsymbol{x}_n \in \mathbb{R}^{P_X}$ and $\boldsymbol{z}_n \in \mathbb{R}^{P_Z}$. Suppose that \boldsymbol{x}_n and \boldsymbol{z}_n are uncorrelated, so that $\mathbb{E}\left[\boldsymbol{x}_n\boldsymbol{z}_n^{\intercal}\right] = \boldsymbol{0}$.

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

b

Now return to the general case. Let $\hat{\beta} = (X^{\mathsf{T}}X)^{-1}X^{\mathsf{T}}Y$ denote the OLS estimator from the regression on X alone. Derive an expression for $\mathbb{E}\left[\hat{\beta}\right]$, where the expectation is taken over X, Y, and Z.

Hint: by the Tower property,

$$\mathbb{E}\left[(\boldsymbol{X}^{\intercal}\boldsymbol{X})^{-1}\boldsymbol{X}^{\intercal}\boldsymbol{Z}\right] = \mathbb{E}\left[(\boldsymbol{X}^{\intercal}\boldsymbol{X})^{-1}\boldsymbol{X}^{\intercal}\mathbb{E}\left[\boldsymbol{Z}|\boldsymbol{X}\right]\right].$$

C

Using (b), derive an expression for the bias for a fixed x_{new} , i.e.

$$\mathbb{E}\left[y_{ ext{new}} - oldsymbol{x}_{ ext{new}}^\intercal \hat{eta} | oldsymbol{x}_{ ext{new}}
ight],$$

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

d

Using your result from (c), show that the predictions are biased at $\boldsymbol{x}_{\text{new}}$ when omitting the variables \boldsymbol{z}_n from the regression precisely when $\gamma^{\intercal}\mathbb{E}\left[\boldsymbol{z}_n|\boldsymbol{x}_n\right]\neq 0$. 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.

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 u and v vectors the same length as A. Then

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

(For reference, I provide a proof in the notes for lecture 21.)

We will also use the following definition of a "leverage score," $h_n := \boldsymbol{x}_n^\intercal (\boldsymbol{X}^\intercal \boldsymbol{X})^{-1} \boldsymbol{x}_n$. We will discuss leverage scores more in the last lecture, but for now it's enough that you know what it is. Note that $h_n = (\boldsymbol{X} (\boldsymbol{X}^\intercal \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal)_{nn}$ is the n-th diagonal entry of the projection matrix $\boldsymbol{P}_{\boldsymbol{X}}$.

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

$$MSE_{LOO} := rac{1}{N} \sum_{n=1}^{N} (y_n - oldsymbol{x}_n^\intercal \hat{oldsymbol{eta}}_{-n})^2.$$

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

Let X_{-n} denote the X matrix with row n left out, and Y_{-n} denote the Y matrix with row n left out.

a

Prove that

$$\hat{\boldsymbol{\beta}}_{-n} = (\boldsymbol{X}_{-n}^\intercal \boldsymbol{X}_{-n})^{-1} \boldsymbol{X}_{-n}^\intercal \boldsymbol{Y}_{-n} = (\boldsymbol{X}^\intercal \boldsymbol{X} - \boldsymbol{x}_n \boldsymbol{x}_n^\intercal)^{-1} (\boldsymbol{X}^\intercal \boldsymbol{Y} - \boldsymbol{x}_n \boldsymbol{y}_n)$$

b

Using the Sherman-Woodbury formula, find an explicit expression for

$$(\boldsymbol{X}^{\intercal}\boldsymbol{X} - \boldsymbol{x}_{n}\boldsymbol{x}_{n}^{\intercal})^{-1}.$$

in terms of \boldsymbol{x}_n , y_n , h_n , and $(\boldsymbol{X}^{\dagger}\boldsymbol{X})^{-1}$.

C

Combine (a) and (b) to derive an explicit expression for $\hat{\boldsymbol{\beta}}_{-n}$ in terms of $\boldsymbol{x}_n, y_n, h_n$, and $(\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X})^{-1}$.

d

Using (c), derive an explicit expression for $\boldsymbol{x}_n^{\mathsf{T}} \hat{\boldsymbol{\beta}}_{-n}$ that depends only on h_n and $\hat{y}_n = \hat{\boldsymbol{\beta}}^{\mathsf{T}} \boldsymbol{x}_n$, where \hat{y}_n is computed using the full dataset without leaving out row n.

е

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 $(\mathbf{X}^{\intercal}\mathbf{X})^{-1}$.

f

Prove that $\sum_{n=1}^{N} h_n = N - P$, and $0 \le h_n \le 1$. Hint: if \boldsymbol{v} is a vector with a 1 in entry n and 0 otherwise, then $h_n = \boldsymbol{v}^{\mathsf{T}} \boldsymbol{P} \boldsymbol{v}$, and projection cannot increase a vector's norm. Recall also that $\operatorname{trace} \left(\boldsymbol{P} \right) = N - P$.

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.