Math 390.4 / 650.3 Spring 2018
Midterm Examination Two

Solutions

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Monday, April 16, 2018

Full Name ____

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Instructions

This exam is 110 minutes and closed-book. You are allowed **one** page (front and back) of a "cheat sheet." You may use a graphing calculator of your choice. Please read the questions carefully. If the question reads "compute," this means the solution will be a number otherwise you can leave the answer in *any* widely accepted mathematical notation which could be resolved to an exact or approximate number with the use of a computer. I advise you to skip problems marked "[Extra Credit]" until you have finished the other questions on the exam, then loop back and plug in all the holes. I also advise you to use pencil. The exam is 100 points total plus extra credit. Partial credit will be granted for incomplete answers on most of the questions. $\boxed{\text{Box}}$ in your final answers. Good luck!

Problem 1 This question is about concepts of OLS.

(a) [4 pt / 4 pts] Solve for $\boldsymbol{c}^\star$ where $B \in \mathbb{R}^{n\times m}$ where $n > m$ and B is full rank:

$$\boldsymbol{c}^\star = \underset{\boldsymbol{c}\in\mathbb{R}^m}{\arg\min} \left\{\boldsymbol{c}^\top B^\top B\boldsymbol{c}\right\}$$

$\Rightarrow \frac{d}{d\vec{c}}\left[\vec{c}^\top B^\top B\vec{c}\right] \overset{\text{set}}{=} \vec{0}$

$\Rightarrow \cancel{2}\, B^\top B\vec{c} = \vec{0}$

since B is full rank $\Rightarrow B^\top B$ is full rank (and square)

$\Rightarrow \underbrace{(B^\top B)^{-1} B^\top B}\vec{c} = \vec{0}\,(B^\top B)^{-1} \Rightarrow \vec{c}^{\,*} = (B^\top B)^{-1}\vec{0} = \boxed{\vec{0}}$

(b) [3 pt / 7 pts] Assume $\boldsymbol{X} \in \mathbb{R}^{n\times(p+1)}$ where $n >> p+1$ and $\boldsymbol{X}$ is full rank and its first column is $\boldsymbol{1}_n$. In terms of $\boldsymbol{X}, n, p$, (1) give an expression for the matrix $\boldsymbol{H}$ which represents the orthogonal projection matrix onto the column space of X, (2) indicate the dimension of the matrix $\boldsymbol{H}$ and (3) indicate the rank of the matrix $\boldsymbol{H}$.

$$\boldsymbol{H} = X(X^\top X)^{-1}X^\top$$

$$\dim[\boldsymbol{H}] = n \times n$$

$$\operatorname{rank}[\boldsymbol{H}] = p+1$$

(c) [8 pt / 15 pts] Assume $\boldsymbol{b}$ is the least squares solution, $\hat{\boldsymbol{y}}$ is the projection of $\boldsymbol{y}$ onto the column space of $\boldsymbol{X}$ defined in (b) via projection matrix $\boldsymbol{H}$ and $\boldsymbol{e}$ is the difference between the original vector and this projection. Simplify the following *as best as possible* or indicate an *illegal operation*.

$\hat{\boldsymbol{y}} \cdot \boldsymbol{e} = 0$

$\hat{\boldsymbol{y}} + \boldsymbol{e} = \vec{y}$

$\hat{\boldsymbol{y}} \cdot \boldsymbol{y} = \vec{\hat{y}} \cdot \vec{y}$ (no simplification)

$\boldsymbol{y} \cdot \boldsymbol{b} =$ illegal operation (since dimensions of the two vectors don't correspond)

$$
\begin{aligned}
\boldsymbol{H}\boldsymbol{H}^\top\hat{\boldsymbol{y}} &= \overset{\text{symmetric}}{H}H\vec{\hat{y}} = \overset{\text{idempotent}}{H}\vec{\hat{y}} = \vec{\hat{y}} \quad \text{already a projection onto colsp}(X) \\
(\boldsymbol{I}-\boldsymbol{H})^\top\hat{\boldsymbol{y}} &= (I^\top - H^\top)\vec{\hat{y}} \overset{\text{symmetric}}{=} (I-H)\vec{\hat{y}} = \vec{\hat{y}} - \vec{\hat{y}} = \vec{0}_n \\
||\boldsymbol{y}||^2 - ||\underbrace{\boldsymbol{X}\boldsymbol{b}}_{\vec{\hat{y}}}||^2 - ||\underbrace{\boldsymbol{y}-\hat{\boldsymbol{y}}}_{\vec{e}}||^2 &= 0 \quad (\text{by Pythagorean thm}) \\
\boldsymbol{H}\begin{bmatrix}\bar{y}\\ \vdots \\ \bar{y}\end{bmatrix} &= H\bar{y}\vec{1}_n = \bar{y}H\vec{1}_n = \bar{y}\vec{1}_n \quad \vec{1}_n \in \text{colsp}(X) \\
\boldsymbol{H}\left[\boldsymbol{1}_n \mid \boldsymbol{x}_{\cdot 4} \mid \boldsymbol{x}_{\cdot 9}\right] &= [\vec{1}_n \mid \vec{x}_{\cdot 4} \mid \vec{x}_{\cdot 9}]
\end{aligned}
$$

since all 3 vectors $\in$ colsp(X)

(d) [6 pt / 21 pts] Assume all notation from (b) and (c). Let $\boldsymbol{X} = \boldsymbol{Q}\boldsymbol{R}$, the Q-R decomposition. Prove that $\boldsymbol{b}$ in the following expression is the standard least squares solution. Show all steps explicitly for full credit.

$$\boldsymbol{R}\boldsymbol{b} = \boldsymbol{Q}^\top\boldsymbol{y}$$

$\Rightarrow QR\vec{b} = QQ^\top\vec{y}$ multiply both sides by Q on the left

$\Rightarrow QR\vec{b} = X(X^\top X)^{-1}X^\top\vec{y}$ since $QQ^\top = H = X(X^\top X)^{-1}X^\top$

$\Rightarrow X\vec{b} = X(X^\top X)^{-1}X^\top\vec{y}$ since $X = QR$

$\Rightarrow X^\top X\vec{b} = \cancel{X^\top X}\cancel{(X^\top X)^{-1}}X^\top\vec{y}$ multiply both sides by $X^\top$ on the left and simplify RHS

$\Rightarrow \cancel{(X^\top X)^{-1}}\cancel{(X^\top X)}\vec{b} = (X^\top X)^{-1}X^\top\vec{y}$ multiply both sides by $(X^\top X)^{-1}$ on the left
note $X^\top X$ is full rank and square so inverse exists
(then simplify)

$\Rightarrow \vec{b} = (X^\top X)^{-1}X^\top\vec{y}$ ✓

(e) [9 pt / 30 pts] Assume all notation means the same as in the previous questions. Now, let $\boldsymbol{X}_{\text{aug}} := [\boldsymbol{X} \mid \boldsymbol{x}_{\text{junk}}]$ where $\boldsymbol{x}_{\text{junk}}$ is a $n \times 1$ vector whose entries are all $\overset{iid}{\sim} \mathcal{N}(0, 1)$. Let the subscript "aug" refer to all quantities of the OLS solution using $\boldsymbol{X}_{\text{aug}}$ instead of $\boldsymbol{X}$. Circle the following statement(s) that are *always* true.

i) $||\boldsymbol{e}||^2 < ||\boldsymbol{e}_{\text{aug}}||^2$

ii) $||\boldsymbol{e}||^2 > ||\boldsymbol{e}_{\text{aug}}||^2$

iii) $||\hat{\boldsymbol{y}}||^2 < ||\hat{\boldsymbol{y}}_{\text{aug}}||^2$

iv) $||\hat{\boldsymbol{y}}||^2 > ||\hat{\boldsymbol{y}}_{\text{aug}}||^2$

v) $||\boldsymbol{y}||^2 < ||\boldsymbol{y}_{\text{aug}}||^2$

vi) $||\boldsymbol{y}||^2 > ||\boldsymbol{y}_{\text{aug}}||^2$

vii) $||\boldsymbol{b}||^2 < ||\boldsymbol{b}_{\text{aug}}||^2$

viii) $||\boldsymbol{b}||^2 > ||\boldsymbol{b}_{\text{aug}}||^2$

ix) $b_{\text{junk}} \approx 0$

x) $R^2 < R^2_{\text{aug}}$

xi) $R^2 > R^2_{\text{aug}}$

~~xii) $||\boldsymbol{y}||^2 < ||\boldsymbol{y}_{\text{aug}}||^2$~~

~~xiii) $||\boldsymbol{y}||^2 > ||\boldsymbol{y}_{\text{aug}}||^2$~~ duplicates

xiv) $\text{rank}[\boldsymbol{H}] > \text{rank}[\boldsymbol{H}_{\text{aug}}]$

xv) $\text{rank}[\boldsymbol{H}] < \text{rank}[\boldsymbol{H}_{\text{aug}}]$

xvi) $x_{\text{junk}} \in \text{colsp}[\boldsymbol{X}_{\text{aug}}]$

xvii) $\hat{\boldsymbol{y}} \in \text{colsp}[\boldsymbol{X}_{\text{aug}}]$

xviii) $\hat{\boldsymbol{y}}_{\text{aug}} \in \text{colsp}[\boldsymbol{X}_{\text{aug}}]$

(f) [4 pt / 34 pts] Assume $\boldsymbol{b}$ is now the least absolute cube solution (not the least squares solution). Simplify the following *as best as possible* or indicate an *illegal operation.*

$\hat{\boldsymbol{y}} \cdot \boldsymbol{e} = \vec{\hat{y}} \cdot \vec{e}$ no simplification possible since the algorithm does not do an orthogonal projection

$\hat{\boldsymbol{y}} + \boldsymbol{e} = \vec{y}$ always true by definition of $\vec{e}$

Problem 2 This question is about the concept of model validation and the strategy we discussed in class.

(a) [6 pt / 40 pts] Let's say we divide scramble the rows of $\mathbb{D}$ then create a partition

$$\mathbb{D} = \begin{bmatrix} \mathbb{D}_{\text{train}} \\ \hline \mathbb{D}_{\text{test}} \end{bmatrix}$$

in a 4:1 ratio train : test (in number of rows). We then fit $g_1 = \mathcal{A}(\mathcal{H}, \mathbb{D}_{\text{train}})$, $g_2 = \mathcal{A}(\mathcal{H}, \mathbb{D}_{\text{test}})$ and $g_{\text{final}} = \mathcal{A}(\mathcal{H}, \mathbb{D})$. Which of the following statement(s) can be employed as a means of *honest* model validation?

i) Comparing $g_1(\boldsymbol{X}_{\text{train}})$ to $\boldsymbol{y}_{\text{train}}$

~~ii) Comparing $g_1(\boldsymbol{X}_{\text{train}})$ to $\boldsymbol{y}_{\text{test}}$~~

iii) Comparing $g_1(\boldsymbol{X}_{\text{test}})$ to $\boldsymbol{y}_{\text{train}}$

iv) Comparing $g_1(\boldsymbol{X}_{\text{test}})$ to $\boldsymbol{y}_{\text{test}}$ what we did in class

v) Comparing $g_2(\boldsymbol{X}_{\text{train}})$ to $\boldsymbol{y}_{\text{train}}$

vi) Comparing $g_2(\boldsymbol{X}_{\text{train}})$ to $\boldsymbol{y}_{\text{test}}$

~~vii) Comparing $g_2(\boldsymbol{X}_{\text{test}})$ to $\boldsymbol{y}_{\text{train}}$~~ by symmetry of the split

viii) Comparing $g_2(\boldsymbol{X}_{\text{test}})$ to $\boldsymbol{y}_{\text{test}}$

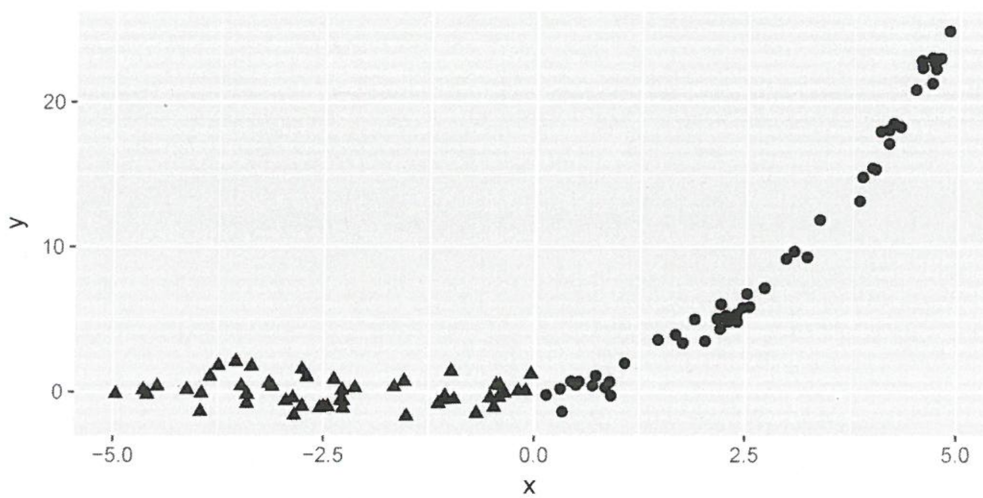
ix) Comparing $g_{\text{final}}(\boldsymbol{X}_{\text{train}})$ to $\boldsymbol{y}_{\text{train}}$

x) Comparing $g_{\text{final}}(\boldsymbol{X}_{\text{train}})$ to $\boldsymbol{y}_{\text{test}}$

xi) Comparing $g_{\text{final}}(\boldsymbol{X}_{\text{test}})$ to $\boldsymbol{y}_{\text{train}}$ using g_{final} is never allowed

xii) Comparing $g_{\text{final}}(\boldsymbol{X}_{\text{test}})$ to $\boldsymbol{y}_{\text{test}}$

Problem 3 This question is about "non-linear" linear modeling. Consider the following data:



Imagine if $\mathbb{D}$ consisted of the subset of the data pictured above where $\mathcal{X} = \{x : x \geq 0\}$ i.e. no triangle points are part of the historical data. Consider $\mathcal{A} = $ OLS and the following model candidate sets:

$$\begin{aligned}\mathcal{H}_1 &= \{w_0 + w_1 x\} \\ \mathcal{H}_2 &= \{w_0 + w_1 x^2\}\end{aligned}$$

(a) [3 pt / 43 pts] Which model candidate set would be better for building a model g using $\mathbb{D}$ whose goal is to predict in $\mathcal{X} = \{0, 3\}$?

i) $\mathcal{H}_1$

ii) $\mathcal{H}_2$ Since the relationship is curved / non linear

iii) not enough information to tell

(b) [3 pt / 46 pts] Which model candidate set would be better for building a model g using $\mathbb{D}$ whose goal is to predict in $\mathcal{X} = \{-3, 3\}$?

i) $\mathcal{H}_1$

ii) $\mathcal{H}_2$

iii) not enough information to tell we would have to run both and see

(c) [3 pt / 49 pts] Which model candidate set would be better for building a model g using $\mathbb{D}$ whose goal is to predict in $\mathcal{X} = \mathbb{R}$?

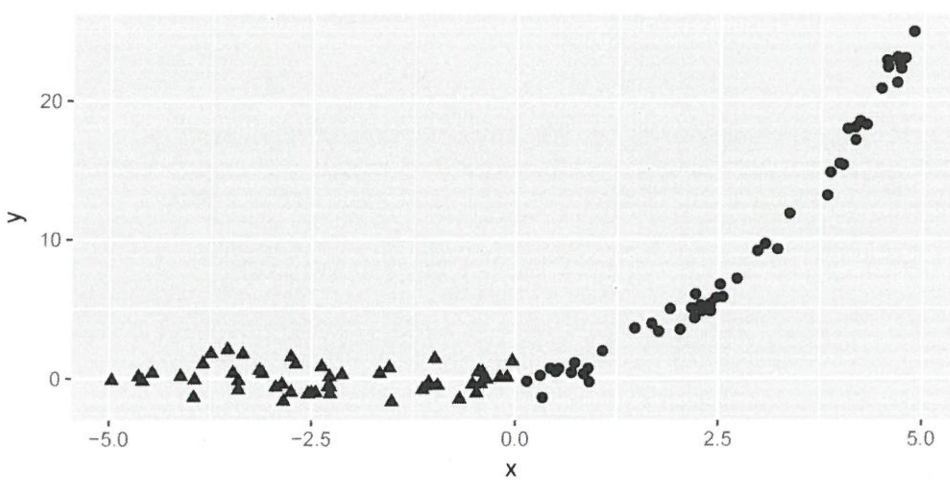
i) $\mathcal{H}_1$

ii) $\mathcal{H}_2$

iii) not enough information to tell

extrapolation beyond range of x provided in $\mathbb{D}$

Problem 4 We continue with "non-linear" linear modeling. We will consider a similar-looking dataset as in the previous problem but the situation will be totally different. Below the response y is plotted by predictor x. However there is a second dummy predictor z which is pictured below as well. If $z = 1$, the illustration displays a circle and if $z = 0$, the illustration displays a triangle. The entire $\mathbb{D}$ is plotted below.



Consider $\mathcal{A} =$ OLS and the following model candidate sets:

$$\begin{aligned}
\mathcal{H}_1 &= \{w_0 + w_1 x\} \\
\mathcal{H}_2 &= \{w_0 + w_1 z\} \\
\mathcal{H}_3 &= \{w_0 + w_1 x^2\} \\
\mathcal{H}_4 &= \{w_0 + w_1 x + w_2 z + w_3 x z\}
\end{aligned}$$

(a) [3 pt / 52 pts] Which model candidate set would be better for building a model g?

i) $\mathcal{H}_1$

ii) $\mathcal{H}_2$

iii) $\mathcal{H}_3$

iv) $\mathcal{H}_4$

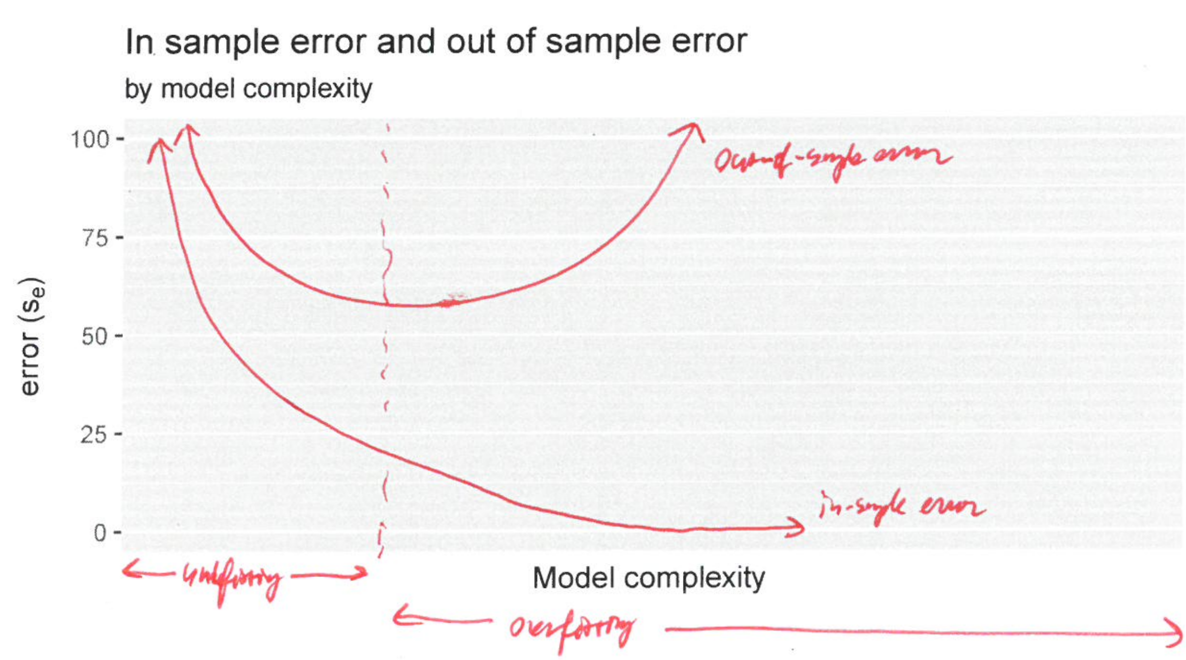
v) not enough information to tell

(b) [6 pt / 58 pts] Regardless of your answer in (a), assume $\mathcal{H}_4$ was employed. Estimate $\boldsymbol{b}$ as best as you can.

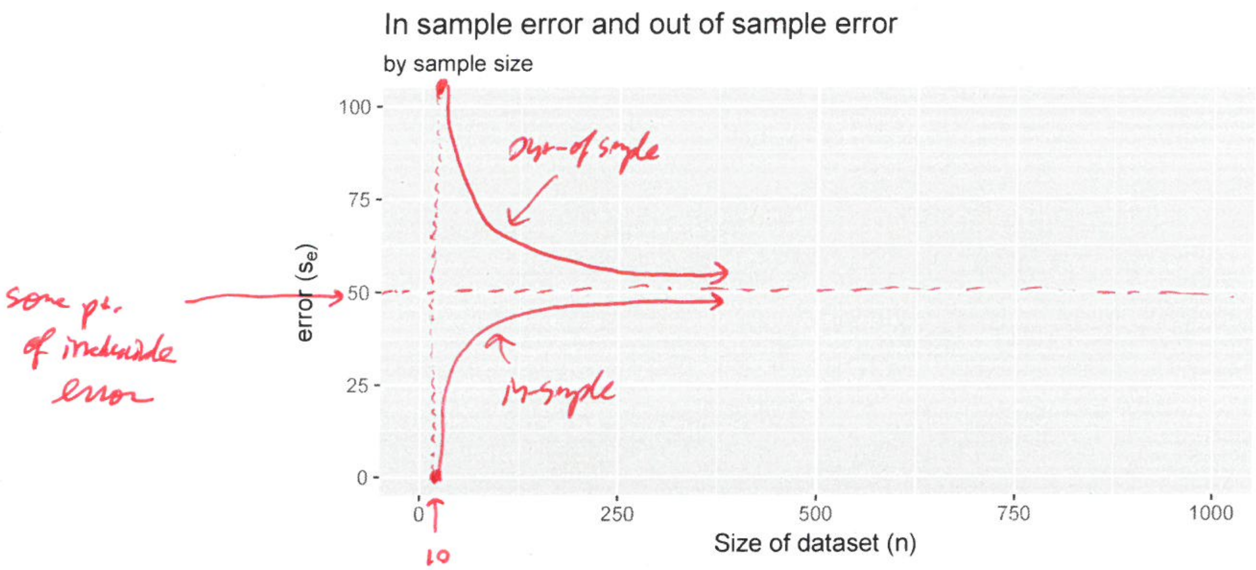
$$\vec{b} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} \approx \begin{bmatrix} 9 \\ 9 \\ 0 \\ 4 \end{bmatrix}$$

Problem 5 This question is about general concepts of modeling including under/overfitting.

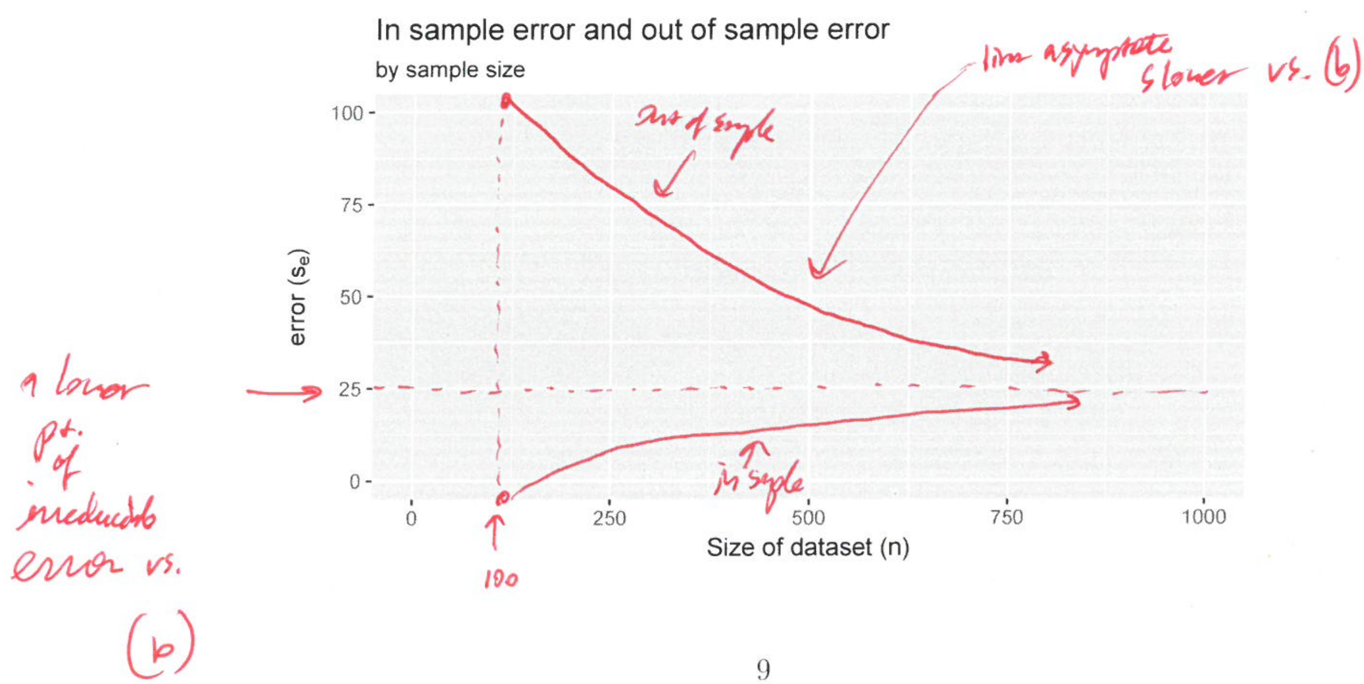
(a) [6 pt / 64 pts] Assume a general $\mathbb{D}$, $\mathcal{A}$ and $\mathcal{H}$ and $\mathcal{Y} \subset \mathbb{R}$. In the graph below, (1) draw the relationship between in-sample error and model complexity, (2) draw the relationship between out-of-sample error and model complexity, then (3) indicate the region of underfitting and (4) indicate the region of overfitting.



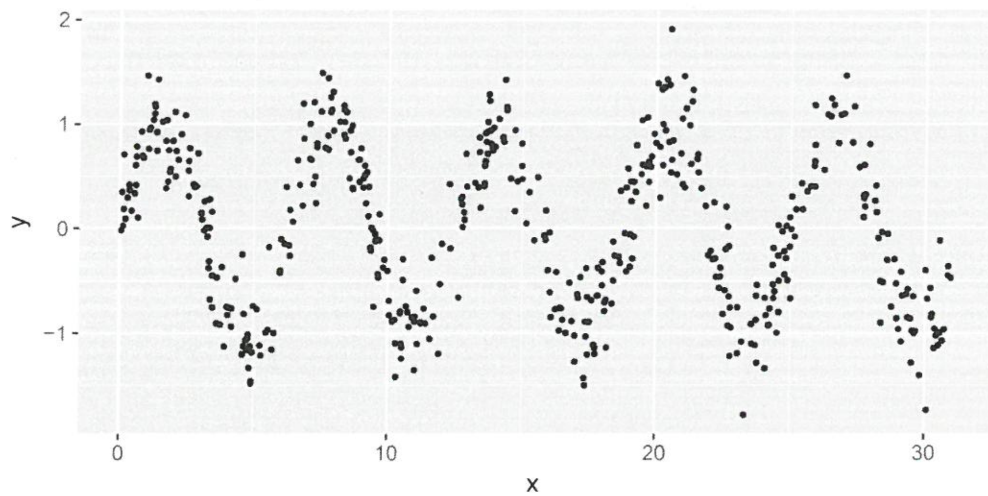
(b) [6 pt / 70 pts] Assume a general phenomenon where you're given $\mathbb{D}$ and $\mathcal{Y} \subset \mathbb{R}$ and $\mathcal{A}$ and corresponds to a least squares minimization for and a simple model space $\mathcal{H}$ with 10 parameters. Assume ϵ is non-zero. Now, (1) draw the relationship between in-sample error and n, the number of data points in $\mathbb{D}$, (2) draw the relationship between out-of-sample error and n.



(c) [3 pt / 73 pts] [Extra credit] Assume the same setup as in (b) but now the model space $\mathcal{H}$ is complex with 100 parameters. Now, (1) draw the relationship between in-sample error and n, the number of data points in $\mathbb{D}$, (2) draw the relationship between out-of-sample error and n. Make sure to indicate clearly how the relationships differ here from the relationships you drew in (b).



(d) [6 pt / 79 pts] Consider the plot below.



Which one(s) of the following statement(s) are most likely true?

i) the predictor x and the response y are correlated

ii) the predictor x and the response y are associated

iii) s_{xy} will be approximately zero

iv) s_{xy} will be exactly zero

v) r will be approximately zero

vi) r will be exactly zero

vii) $\delta = 0$

viii) $f(x) = 0$

ix) the random variable X (that generated the realizations of x above) and the random variable Y (that generated the $\overset{iid}{\sim}$ realizations of y) are dependent

x) the random variable X (that generated the realizations of x above) and the random variable Y (that generated the $\overset{iid}{\sim}$ realizations of y) are independent

xi) this data is only of theoretical interest and can never be found in the real world

xii) a linear model with polynomial terms will take many degrees of freedom to fit well

xiii) a model with a intelligently selected $\mathcal{H}$ can be fit with very few degrees of freedom

xiv) this data can *only* be fit if one uses three splits of $\mathbb{D}$ — one for training, one for selection and one for testing

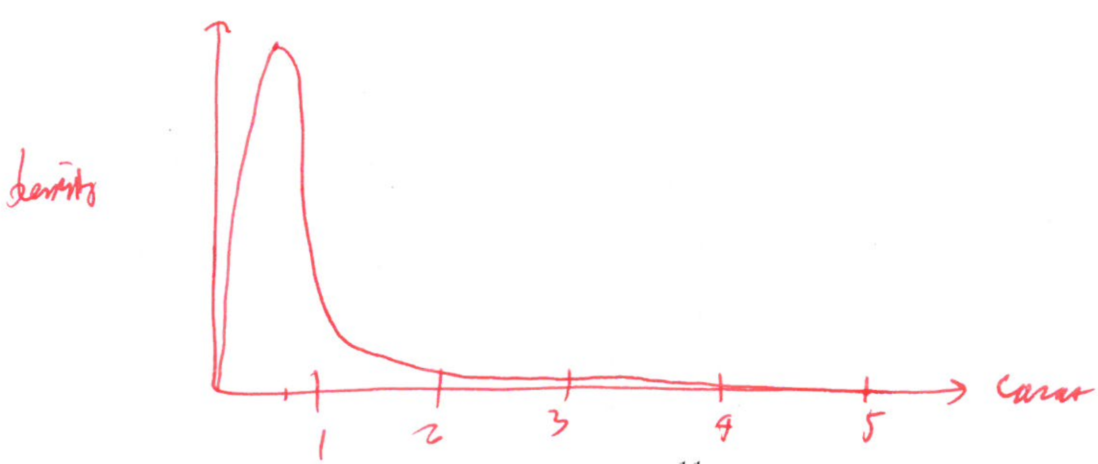
Problem 6 Below are some questions on the practice topics we studied. We first load the diamonds data and we remind ourselves of the response (`price`) and the 9 features:

```
> pacman::p_load(ggplot2)
> data(diamonds)
> diamonds$cut = factor(as.character(diamonds$cut))
> diamonds$color = factor(as.character(diamonds$color))
> diamonds$clarity = factor(as.character(diamonds$clarity))
> summary(diamonds)
     carat             cut            color        clarity
 Min.   :0.2000   Fair     : 1610   D: 6775   SI1    :13065
 1st Qu.:0.4000   Good     : 4906   E: 9797   VS2    :12258
 Median :0.7000   Ideal    :21551   F: 9542   SI2    : 9194
 Mean   :0.7979   Premium  :13791   G:11292   VS1    : 8171
 3rd Qu.:1.0400   Very Good:12082   H: 8304   VVS2   : 5066
 Max.   :5.0100                     I: 5422   VVS1   : 3655
                                    J: 2808   (Other): 2531
     depth           table           price             x
 Min.   :43.00   Min.   :43.00   Min.   :  326   Min.   : 0.000
 1st Qu.:61.00   1st Qu.:56.00   1st Qu.:  950   1st Qu.: 4.710
 Median :61.80   Median :57.00   Median : 2401   Median : 5.700
 Mean   :61.75   Mean   :57.46   Mean   : 3933   Mean   : 5.731
 3rd Qu.:62.50   3rd Qu.:59.00   3rd Qu.: 5324   3rd Qu.: 6.540
 Max.   :79.00   Max.   :95.00   Max.   :18823   Max.   :10.740

       y                z
 Min.   : 0.000   Min.   : 0.000
 1st Qu.: 4.720   1st Qu.: 2.910
 Median : 5.710   Median : 3.530
 Mean   : 5.735   Mean   : 3.539
 3rd Qu.: 6.540   3rd Qu.: 4.040
 Max.   :58.900   Max.   :31.800
```

(a) [4 pt / 83 pts] As best as you can, illustrate the output of the following code. Make sure you label axes and provide some tick marks.

```
> ggplot(diamonds) +
    geom_density(aes(carat))
```



(b) [4 pt / 87 pts] We now run an anova model as follows:

```
> anova_mod = lm(price ~ cut, diamonds)
```

and below are the $\boldsymbol{b}$ and RMSE:

```
> coef(anova_mod)
 (Intercept)       cutGood      cutIdeal   cutPremium cutVery Good
   4358.7578     -429.8933     -901.2158     225.4999    -376.9979
> summary(anova_mod)$sigma
[1] 3963.847
```

The first six entries of the variable `cut` are:

```
> head(diamonds$cut)
[1] Ideal     Premium   Good      Premium   Good      Very Good
Levels: Fair Good Ideal Premium Very Good
```

Provide below the first six rows of the model matrix $\boldsymbol{X}$ for the model `price` $\sim$ `cut`.

(Intercept)	cut-good	cut-ideal	cut-premium	cut-verygood
1	0	1	0	0
1	0	0	1	0
1	1	0	0	0
1	0	0	1	0
1	1	0	0	0
1	0	0	0	1

(c) [3 pt / 90 pts] [Extra credit] Given the model and the results in (b), illustrate as best as you can the result of the following code. Credit will only be given to near perfect renditions.

```
> ggplot(diamonds) +
    geom_boxplot(aes(x = cut, y = price))
```

(d) [6 pt / 96 pts] The first six entries of carat are

```
> head(diamonds$carat)
[1] 0.23 0.21 0.23 0.29 0.31 0.24
```

Illustrate the result of the following code:

```
> head(model.matrix(price ~ carat * cut, diamonds))
```

(Intercept)	carat	cut-good	cut-ideal	cut-premium	cut-very-good	carat: cut-good	carat: cut-ideal	carat: cut-premium	carat: cut-very-good
1	0.23	0	1	0	0	0	0.23	0	0
1	0.21	0	0	1	0	0	0	0.21	0
1	0.23	1	0	0	0	0.23	0	0	0
1	0.29	0	0	1	0	0	0	0.29	0
1	0.31	1	0	0	0	0.31	0	0	0
1	0.24	0	0	0	1	0	0	0	0.24

(e) [6 pt / 102 pts] Consider $\mathcal{A}$ = OLS and the following models explaining diamond `price`:

1. a 4-degree polynomial of carat
2. all raw features
3. all features interacted with carat
4. all interactions

Write code below to fit these four models and save them as `mod_1`, `mod_2`, `mod_3`, `mod_4`.

attach(diamonds) or put ", diamonds" here

mod_1 = lm(price ~ poly(carat, 4))

mod_2 = lm(price ~ .)

mod_3 = lm(price ~ carat * .)

mod_4 = lm(price ~ . * .)

(f) [4 pt / 106 pts] If R^2 was employed to select the "best" model of the four in (d), what would be the result? That is, which model would it declare the winner?

Model # 4

(g) [5 pt / 111 pts] [Extra credit] Write code below that will select the "best" model of the four in (d) as measured by future predictive performance.