STAT 343 Homework 8 Aaron Maurer

1. (a) As we have proved, if the matix X isn't singular, then the least squares solution from OLS is unique and indeed the optimal fit. Thus, if a  $\beta$  acheives the minimum least squares, it must be the OLS coefficient from the regression. Calculating the sum of squares for a coefficient  $\hat{\beta}^{(-i)}$  on  $\tilde{Y}^{(-i)}$ , we get

$$\|\tilde{Y}^{(-i)} - X\hat{\beta}^{(-i)}\|^2 = (x_i\beta^{(-i)} - x_i\beta^{(-i)})^2 + \|Y^{(-i)} - X^{(-i)}\hat{\beta}^{(-i)}\|^2$$
$$\|\tilde{Y}^{(-i)} - X\hat{\beta}^{(-i)}\|^2 = \|Y^{(-i)} - X^{(-i)}\hat{\beta}^{(-i)}\|^2$$

Since the sum on the right is the minimum possible over all  $\beta$  (since the coefficient was fit by OLS on  $Y^{(-i)}$ ),  $\hat{\beta}^{(-i)}$  minimizes the sum of squares for  $\tilde{Y}^{(-i)}$ . By our earlier reasoning, it thus must be the coefficient that would result from OLS run predicting  $\tilde{Y}^{(-i)}$  in terms of X.

- (b) The prediction of a linear model with coefficient  $\hat{\beta}^{(-i)}$  at point  $x_i^T$  is  $x_i^T \hat{\beta}^{(-i)}$ , so since that is the coefficient for regressing  $\tilde{Y}^{(-i)}$  on X,  $x_i^T \hat{\beta}^{(-i)}$  will be the fit.
- 2. (a)

$$\hat{y}_{i} - \hat{f}^{(-i)}(x_{i}) = y_{i} - S(x_{i})^{(-i)}Y^{(-i)}$$

$$\hat{y}_{i} - \hat{f}^{(-i)}(x_{i}) = y_{i} - \frac{1}{\sum_{j \neq i} S_{ij}} \sum_{j \neq i} y_{j}S_{ij}$$

$$\hat{y}_{i} - \hat{f}^{(-i)}(x_{i}) = y_{i} - \frac{\hat{f}(x_{i}) - y_{i}S_{ii}(X)}{1 - S_{ii}}$$

$$\hat{y}_{i} - \hat{f}^{(-i)}(x_{i}) = \frac{y_{i} - y_{i}S_{ii} - \hat{f}(x) + y_{i}S_{ii}}{1 - S_{ii}}$$

$$\hat{y}_{i} - \hat{f}^{(-i)}(x_{i}) = \frac{y_{i} - \hat{f}(x)}{1 - S_{ii}}$$

- (b) Rather than refitting the regression n times to estimate the leave one out cross validation estimate of error, this allows the regression to merely be fit once, saving a lot of costly QR factorization or matrix inversion.
- (c) Since  $1 \ge 1 S_{ii} \ge 0$ , we have

$$|y_{i} - \hat{f}(x_{i})| \leq \frac{|y_{i} - \hat{f}(x_{i})|}{1 - S_{ii}}$$

$$|y_{i} - \hat{f}(x_{i})| \leq \left| \frac{y_{i} - \hat{f}(x_{i})}{1 - S_{ii}} \right|$$

$$|y_{i} - \hat{f}(x_{i})| \leq \left| y_{i} - \hat{f}^{(-i)}(x_{i}) \right|$$

3. (a) Applying backwards elimination with a critical value of .2, we only remove the variable status. After that, all predictors have a p-value of less than .2, so we stop.

p-value at the point of exclusion:

	Order	p-value
status	1.000	0.853

Resulting model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	24.139	14.769	1.634	0.109
sex	-22.960	6.771	-3.391	0.002
income	4.898	0.955	5.128	0.000
verbal	-2.747	1.825	-1.505	0.140

(b) For each of the following three methods, I used an exhaustive subset search, which determined which set of a particular number of variables resulted in the smallest RSS. The result, which is a boolean indicating whether the predictor should be included at each number of predictors is below. Since this will uniformly be the best model of n predictors, the remaining decision is which n to use. It should be noted that the model in a is indeed the optimal model of 3 predictors.

	(Intercept)	sex	status	income	verbal
1	TRUE	FALSE	FALSE	TRUE	FALSE
2	TRUE	TRUE	FALSE	TRUE	FALSE
3	TRUE	TRUE	FALSE	TRUE	TRUE
4	TRUE	TRUE	TRUE	TRUE	TRUE

The model with the lowest AIC also had 3 predictors, and is thus the same as in a. The different AICs for the best model with n predictors below.

	1	2	3	4
Predictors	1.000	2.000	3.000	4.000
AIC	304.336	296.627	296.214	298.176

(c) The model with the highest adjusted  $\mathbb{R}^2$  is this same model with 3 predictors. Optimal adjusted  $\mathbb{R}^2$  for different number of predictors are below.

	1	2	3	4
Predictors	1.000	2.000	3.000	4.000
Adjusted R Squared	0.373	0.479	0.493	0.482

(d) Going by Mallow's  $C_p$ , we once again get the same model. The smallest model that had a  $C_p$  smaller than the number of parameters (one more than the number of predictors due to the intercept) was the model with 3 predictors (4 parameters):

	1	2	3	4
Parameters	2.000	3.000	4.000	5.000
Mallow's Cp	11.401	3.248	3.035	5.000

4. The order of these operations doesn't make much difference. Point 21 is influential both before and after model selection, and the prefered model includes Air.Flow and Water.Temp, while excluding Acid.Conc, whether or not the outlier is included.

Our initial model is below. Acid. Conc looks ripe to be removed with a high p-value

	Estimate	Std. Error	t value	$\Pr(> t )$
(Intercept)	-39.920	11.896	-3.356	0.004
Air.Flow	0.716	0.135	5.307	0.000
Water.Temp	1.295	0.368	3.520	0.003
Acid.Conc.	-0.152	0.156	-0.973	0.344

Indeed, when we test all subsets of the data, it is excluded from every model that has fewer than three predictors:

-	(Intercept)	Air.Flow	Water.Temp	Acid.Conc.
1	TRUE	TRUE	FALSE	FALSE
2	TRUE	TRUE	TRUE	FALSE
3	TRUE	TRUE	TRUE	TRUE

The optimal subset, when going by adjusted  $R^2$  is the model with just two predictors ( $R^2$  for each optimal subset of a particular size below):

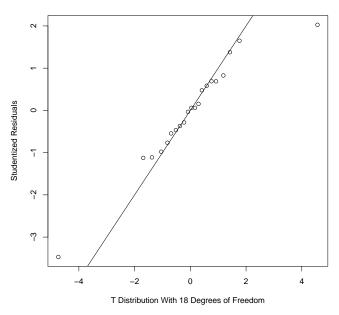
	X
1	0.838
2	0.899
3	0.898

Choosing this as our model, we get the following model:

	Estimate	Std. Error	t value	$\Pr(> t )$
(Intercept)	-50.359	5.138	-9.801	0.000
Air.Flow	0.671	0.127	5.298	0.000
Water.Temp	1.295	0.367	3.525	0.002

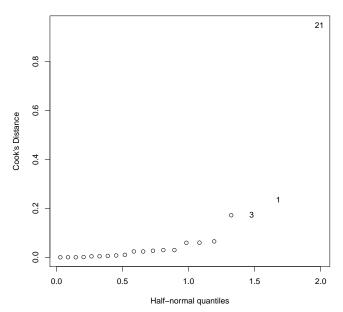
Checking the distribution of studentized residuals for outliers, we see one potential culprit (the largest residual, in the top right, which heavily deviates from T-distribution).

QQ Plot Studentized Resisduals vs. T Distribution



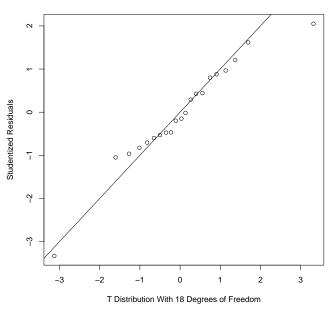
It is the 21st data point. With a studentized residual value of -3.47, it is just inside conservative Bonferroni critical value, for  $\alpha = .5$ , of -3.53. Thus, we don't quite reject it as an outlier. However, looking at the plot of Cook's distances, it is clear that the same point is highly influential.





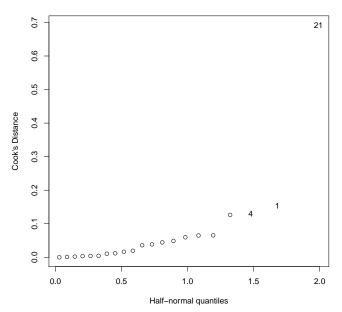
Now, going back to the full model which included Acid.Conc, we look again for outliers and influential points. Shockingly, the same point is once again the only real canidate. The distribution of studentized residuals on this





Testing it as an outlier as before, it has a studentized residual of -3.33 in this model, while the critical value is -3.54, so we don't reject it. However, its still influential, so we kick it out for that:

## Halfnorm Cook's Distances



Preforming variable selection on the data set with this point excluded, we still find the optimal model has the two variables besides Acid.Conc. Optimal subsets of each size:

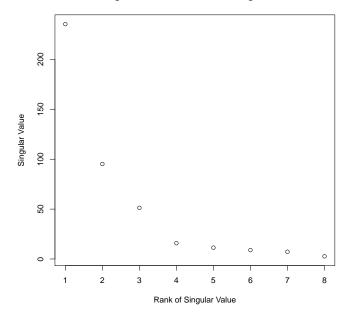
	(Intercept)	Air.Flow	Water.Temp	Acid.Conc.
1	TRUE	TRUE	FALSE	FALSE
2	TRUE	TRUE	TRUE	FALSE
3	TRUE	TRUE	TRUE	TRUE

Adjusted  $R^2$  for these subsets, showing we still prefer the model with two predictors:

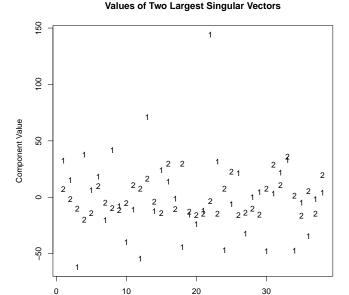
	X
1	0.923
2	0.940
3	0.939

5. (a) I have plotted the singular values below, gotten by taking the square roots of the absolute values of the eigenvalues of  $XX^T$  (once X had been centered). They quickly fall off to very small values, reflecting that most of the variation in the data set is explained by just a few underlying components.

## Singular Values of Centered Design Matrix



(b) The components of the two largest singular vectors are plotted below. As would be expected, the components of the second vector are generally far smaller than those of the first. It appears that approximately half the time the second component has the same sign as the first, and half the time the opposite sign, as might be expected since they are orthogonal. The vaguely resemble piecies of orthogonal waves.



(c) We see that the regression on the two largest principle components doesn't actually predict the data as well as the two best predictors from the original data set (for the same number of variables, the latter has higher  $R^2$ ). While this latter model predicts almost as well as the model including all variables, the largest principle components are signficantly less predictive, though still reasonably predictive. The reason for this is that the principle components are a decomposition of variation within the predictors; however, the largest source of variation in these predictors isn't necessarily predictive of the outcome. For instance, if there is a lot of variation among a few variables that aren't predictive of the outcome, they may correspond to large principle components, but these principle components will likely be also unpredictive. On the other hand, since the principle components as a whole define a space equivalent to

Vector Component

the orignal space defined by all the predictors, a model including all of them will be equally predictive to including all variables.

The regression on the two largest principle components ( $R^2 = .5469$ ):

	Estimate	Std. Error	t value	$\Pr(> t )$
(Intercept)	-164.885	6.697	-24.622	0.000
PCPC1	-1.049	0.175	-5.984	0.000
PCPC2	1.099	0.433	2.537	0.016

The regression on all variables  $(R^2 = .6866)$ :

	Estimate	Std. Error	t value	$\Pr(> t )$
(Intercept)	436.432	166.572	2.620	0.014
Age	0.776	0.570	1.360	0.184
Weight	0.026	0.331	0.080	0.937
HtShoes	-2.692	9.753	-0.276	0.784
$\operatorname{Ht}$	0.601	10.130	0.059	0.953
Seated	0.534	3.762	0.142	0.888
$\operatorname{Arm}$	-1.328	3.900	-0.341	0.736
Thigh	-1.143	2.660	-0.430	0.671
Leg	-6.439	4.714	-1.366	0.182

The regression on age and height  $(R^2 = .6562)$ :

	Estimate	Std. Error	t value	$\Pr(> t )$
(Intercept)	526.959	92.248	5.712	0.000
Age	0.521	0.386	1.349	0.186
$\operatorname{Ht}$	-4.200	0.531	-7.906	0.000