STATS305A - Lecture 11

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Contents

1 Announcements

- Homework 2 due today.
- Etude 2 due on Thursday.

2 Leverage

In the linear model $Y = X\beta + \varepsilon$, we define $H = X(X^TX)^{-1}X^T$ and we define

$$H_{ii} = i^{th} \text{ diagonal entry of } H = i^{th} \text{ leverage score.}$$

We have seen multiple interpretations of leverage score:

- Self influence of example i on itself.
- $\frac{\partial \widehat{y}_i}{\partial y_i} = H_{ii}$.

We also have the leave one out calculation. We saw that if $\widehat{y}_{\setminus i} = x_i^T \widehat{\beta}_{\setminus j}$ where $\widehat{\beta}_{\setminus i} = (X_{\setminus i}^T X_{\setminus i})^{-1} X_{\setminus i}^T Y_{\setminus i}$ and

$$X_{\setminus i} = [x_j^T]_{j \neq i} \in \mathbb{R}^{(n-1)\times d} \quad \text{and} \quad Y_{\setminus i} = [Y_j]_{j \neq i} \in \mathbb{R}^{n-1},$$

then

$$\widehat{y}_i = x_i^T \widehat{\beta} = (1 - H_{ii})\widehat{y}_{\setminus i} + H_{ii} y_i.$$

Thus (since $H_{ii} \in [0,1]$), $\widehat{y}_i$ is a convex combination of $\widehat{y}_{\setminus i}$ and y_i. This also gives us a way to effeciently calculate every $\widehat{y}_{\setminus i}$. This is something special about the linear model. Note that if we rearrange the above expression we get

$$\widehat{y}_{\setminus i} = \frac{1}{1-H_{ii}}\widehat{y}_i - \frac{H_{ii}}{1-H_{ii}}y_i,$$

Thus

$$[\widehat{y}_{\setminus i}]_{i=1}^n = \operatorname{diag}(I-H)^{-1}\left(\widehat{y} - \operatorname{diag}(H)y\right).$$

Thus in $O(n)$ times we can do *all* leave one out predictions assuming that we have the matrix H.

3 Residuals, variance and leverage score

Recall $\widehat{\varepsilon} = Y - \widehat{Y} = (I-H)Y$. We always have $\widehat{\varepsilon}^T\widehat{Y} = 0$. This is because

$$\widehat{\varepsilon}^T\widehat{Y} = \widehat{Y}^T(I-H)H\widehat{Y} = \widehat{Y}^T(H-H)\widehat{Y} = 0.$$

The intepretation is that $\widehat{\varepsilon}$ is the noise after removing all "information" in the directions of range(X) and $\widehat{Y}$ is the expected value of Y in the X directions.

Now suppose we have the distributional assumptions $Y = X\beta + \varepsilon$ where $\varepsilon \sim (0, \sigma^2 I)$. We then have $\widehat{\varepsilon} \sim (0, \sigma^2(I-H))$ and so

$$\operatorname{cov}(\widehat{\varepsilon}_i, \widehat{\varepsilon}_j) = \begin{cases} \sigma^2(1-H_{ii}) & \text{if } i = j, \\ -\sigma^2 H_{ij} & \text{else.} \end{cases}$$

And

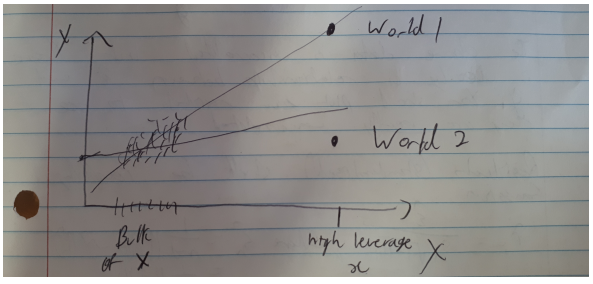
$$\operatorname{Cov}(\widehat{y}, \widehat{\varepsilon}) = 0.$$

Thus the residuals are typically correlated even when have noise $\varepsilon \sim (0, \sigma^2 I)$ (in this case we say that the noise is *homoscedastic*). Note also that

$$\operatorname{Var}(\widehat{\varepsilon}_i) = \sigma^2(1-H_{ii}) \leq \sigma^2 = \operatorname{Var}(\varepsilon_i).$$

We call the above decrease in variance, *variance deflation*. The larger the leverage score, the more deflation we have.

Recall the below picture and our intuition that a point with high leverage may be problematic and that the high leverage points are characterized by x_i being far from the "bulk" of X. If we have a point of high leverage x_i, then we could imagine two worlds with different values of y_i. Since x_i is high leverage, the point $\widehat{y}_i = x_i^T\widehat{\beta}$ changes a lot as y_i changes. This means that our model is more sensitive to changes in y_i than changes in y at points with low leverage.



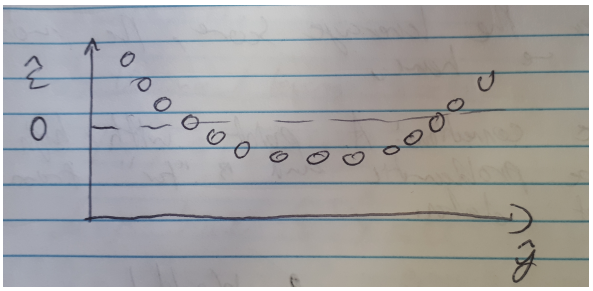
4 Plots and diagnostics

How do we decide if our linear models are "good enough"? We have a number of possible desiderata. Some plots which are good sanity checkes

- Residuals vs fitted values.
- Residuals vs individual features ie columns in X.
- Residuals vs quantiles of Gaussians called a QQ or quantile quantile plot.

4.1 Residuals vs predicted values

One is that the residual $\widehat{\varepsilon}$ should be *really* uncorrelated with the predicted values $\widehat{y}$. Consider the below plot:



The above data is uncorrelated but there is clear a relationship between $\widehat{\varepsilon}$ and $\widehat{y}$. You should always plot your residuals against your predicted values to see they are *really* uncorrelated. In the above example we can conclude that the linear model is probably false and we really want to include a term of the form $(x^T\beta)^2$ in our model. Unfortunately this make our model non-linear and there's not much we can do.

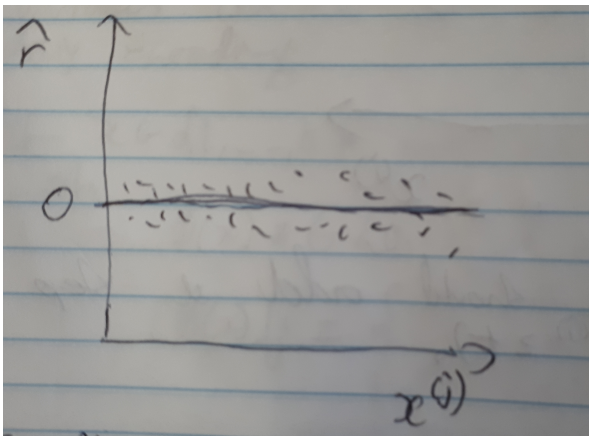
The standardized residuals should be roughly Gaussian. That is define

$$\widehat{r}_i = \frac{\widehat{\varepsilon}_i}{S_n\sqrt{1-H_{ii}}},$$

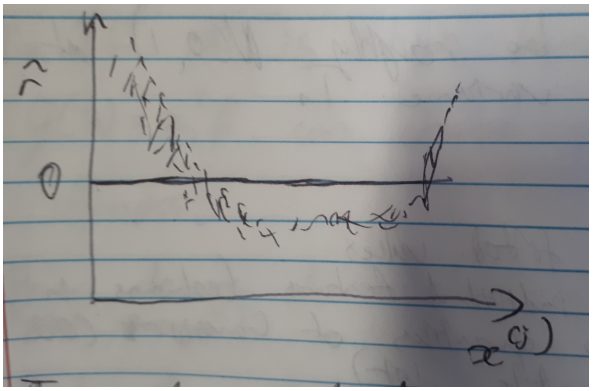
where $S_n^2 = \frac{1}{n-d}\|X\beta - Y\|_2^2 = \frac{1}{n-d}\|\widehat{\varepsilon}\|_2^2$. These normalized residuals should be rouhgly $\mathsf{N}(0,1)$ at least they should have variance 1.

4.2 Residuals vs features

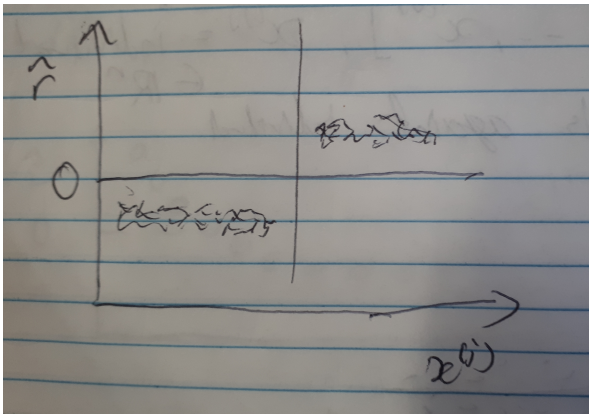
Suppose $X = [x^{(1)}, \ldots, x^{(d)}]$ so $x^{(j)} \in \mathbb{R}^n$ is an individual feature. We could plot the residuals against the individual features. We might get a plot like this:



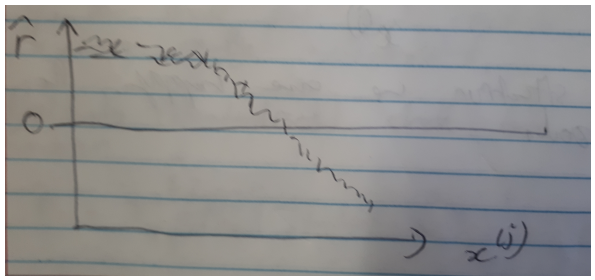
In this situation we are happy and the relationship between the residuals and the feature looks good. We might also have:



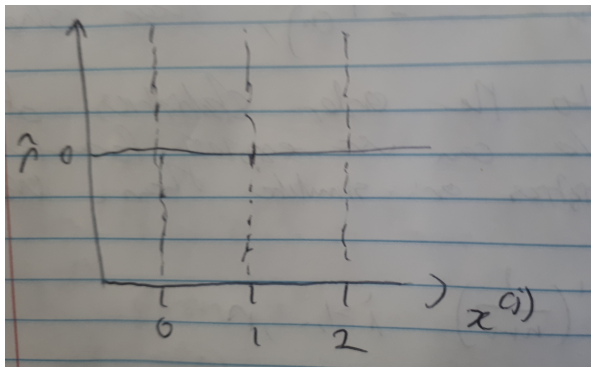
This suggest we should add a polynomial feature like $(x^{(j)})^2$ to our model. We might also have



In which case we should add a feature which is a step function like $\mathbf{1}(x^{(j)} > t)$ where $\mathbf{1}(A)$ is the indicator function of A. We might have



In this case we should add $(x^{(j)} - t)_+$, the positive part of $x^{(j)} - t$. Lastly we might have



Which means that $x^{(j)}$ is a categorical variable and we should not included it "raw" in our model. We should re-encode the variable. There are many names for this re-encoding such as one-hot encoding, dummy variables, factors, $\{0,1\}$-encoding. These all refer to the same process:

If $x \in \{1, \ldots, k\}$, we replace x with $\phi(x) \in \{0,1\}^k$ given by

$$[\phi(x)]_j = \begin{cases} 1 & \text{if } x = j, \\ 0 & \text{else.} \end{cases}$$

This is similiar to the encoding used for k-groups ANOVA.

4.3 QQ Plots

Idea: We can compare the quantiles of $\widehat{r}_i = \frac{\widehat{\varepsilon}_i}{S_n\sqrt{1-H_{ii}}}$ to the quantiles of a standard normal. First we sort the standized residuals $\widehat{r}_{(1)} \leq \widehat{r}_{(2)} \leq \ldots \leq \widehat{r}_{(n)}$, these should be similiar to the order statistics of a Gaussian. We could use analytic formulas for these order statistics or simulate them. In practice we can also use

$$v_{(i)} = \Phi^{-1}\left(\frac{i}{n+1}\right), \quad \text{for } i = 1, \ldots, n.$$

We would then expect $v_{(i)} \approx \widehat{r}_{(i)}$.

4.4 Added variable plot

These give us a sense of how much a variable adds to a model when "adjusting" for other variables.

The mathematical insight: Suppose $X = [x^{(1)}, \ldots, x^{(d)}]$, then the component of $\widehat{\beta}_j$ in ordinary least squares is equal to the regression of y on $x^{(j)}$ adjusting for other variables.

By adjusting we mean we first do regression on $x^{(j)}$ using all the other variables then we subtract this and take $\widehat{x}^{(j)}$ to be what's left. Then we use $\widehat{x}^{(j)}$ to do regression on y.

Let's prove this for $\widehat{\beta}_d$. Suppose $X = QR$ where $Q \in \mathbb{R}^{n\times d}$ satisfies $Q^TQ = I_d$ and $R \in \mathbb{R}^{d\times d}$ is invertible and upper triangular. Write $Q = [q_1, \dots, q_d]$. We know from Gram-Schmidt that if

$$\widehat{x}^{(d)} = x^{(d)} - \sum_{j=1}^{d-1} q_j \langle q_j, x^{(d)}\rangle = (I_n - Q_{\setminus d}Q_{\setminus d}^T)x^{(d)},$$

then $\widehat{x}^{(d)}$ is orthogonal to q_j for $j < d$. Thus we can think of $\widehat{x}^{(d)}$ as what is left from $x^{(d)}$ after taking away the information in the other variables. We can think of $\widehat{x}^{(d)}$ as $x^{(d)}$ with the "best prediction" of $x^{(d)}$ from $x^{(1)}, \dots x^{(d-1)}$ removed. We say $\widehat{x}^{(d)}$ is $x^{(d)}$ *adjusted for* $x^{(1)}, \dots, x^{(d-1)}$.

Recall that $q_d = \frac{\widehat{x}^{(d)}}{\left\|\widehat{x}^{(d)}\right\|_2}$ and $R_{dd} = \left\|\widehat{x}^{(d)}\right\|_2$. Let's solve the normal equations. Note that

$$\begin{aligned} X^TX\beta = X^TY &\iff R^TQ^TQR\beta = R^TQ^TY \\ &\iff R\beta = Q^TY. \end{aligned}$$

Thus if we look at the d^{th} component, we see that $\widehat{\beta}_d$ must solve $R_{dd}\beta_d = q_d^Ty$. Thus

$$\widehat{\beta}_d = \frac{(\widehat{x}^{(d)})^Ty}{\left\|\widehat{x}^{(d)}\right\|_2^2}.$$

Now consider one dimensional linear regression of y on $z \in \mathbb{R}$. We wish to find

$$\min_{b\in\mathbb{R}} \sum_{i=1}^n (y_i - z_ib)^2.$$

The minimizer b^* satisfies $\sum_{i=1}^n z_iy_i = \left(\sum_{i=1}^n z_i^2\right) b^*$ and so $b^* = \frac{z^Ty}{\|z\|_2^2}$.

Upshot: $\widehat{\beta}_j$ is the regression of y onto $x^{(j)}$ adjusting for $x^{(k)}$ for all $k \neq j$.This gives us an idea of something to plot. If we wish to see if the variable j should be included in our model we can plot y adjusted for $x^{(k)}$ for $k \neq j$ against $\widehat{x}^{(j)}$. We can then look for a strong linear relationship in the plot. If their is a strong relationship we should include $x^{(j)}$.