Residuals and Diagnostics

STA 721: Lecture 21

Merlise Clyde
Duke University

Linear Model Assumptions

Linear Model:

$$\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

Assumptions:

$$\boldsymbol{\mu} \in C(\mathbf{X}) \Leftrightarrow \boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$$
$$\boldsymbol{\epsilon} \sim \textsf{N}(\mathbf{0}_n, \sigma^2 \mathbf{I}_n)$$

Focus on

- Wrong mean for a case or cases
- Cases that influence the estimates of the mean
- Wrong distribution for $\boldsymbol{\epsilon}$

If $\mu_i \neq \mathbf{x}_i^T \boldsymbol{\beta}$ then expected value of $e_i = Y_i - \hat{Y}_i$ is not zero

Standardized residuals

- Standardized residuals $e_i/\sqrt{\sigma^2(1-h_{ii})}$
- h_{ii} is the ith diagonal element of the hat matrix $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ or *leverage*
- Under correct model standardized residuals have mean 0 and scale 1
- plug in the usual unbiased estimate of σ^2

$$r_i = e_i/\sqrt{\hat{\sigma}^2(1-h_{ii})}$$

- if h_{ii} is close to 1, then $\hat{Y}_i$ is close to Y_i (why?!?) so e_i is approximately 0
- var(e_i) is also almost 0 as $h_{ii} \to 1$, so $e_i \to 0$ with probability 1
- if $h_{ii} \approx 1$ r_i may not flag ``outliers"
- even if h_{ii} is not close to 1, the distribution of r_i is not a t (hard to judge if large $|r_i|$ is unusual)

Outlier Test for Mean Shift

Test H_0: $\mu_i = \mathbf{x}_i^T \boldsymbol{\beta}$ versus H_a: $\mu_i = \mathbf{x}_i^T \boldsymbol{\beta} + \alpha_i$

- t-test for testing H$_0$: $\alpha_i = 0$ has $n - p - 1$ degrees of freedom
- if p-value is small declare the ith case to be an outlier: E$[Y_i]$ not given by $\mathbf{X}\boldsymbol{\beta}$ but $\mathbf{X}\boldsymbol{\beta} + \delta_i \alpha_i$
- Can extend to include multiple δ_i and δ_j to test that case i and j are both outliers
- Extreme case $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta} + \mathbf{I}_n \boldsymbol{\alpha}$ all points have their own mean!
- Need to control for multiple testing without prior reason to expect a case to be an outlier (or use a Bayesian approach)

Predicted Residuals

Estimates without Case (i):

$$\begin{aligned}\hat{\boldsymbol{\beta}}_{(i)} &= (\mathbf{X}_{(i)}^T \mathbf{X}_{(i)})^{-1} \mathbf{X}_{(i)}^T \mathbf{Y}_{(i)} \\ &= \hat{\boldsymbol{\beta}} - \frac{(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i e_i}{1 - h_{ii}}\end{aligned}$$

How to Calculate $\hat{\beta}_{(i)}$

How do we calculate $\hat{\boldsymbol{\beta}}_{(i)}$ without case i without refitting the model n times?

- Note: $\mathbf{X}^T\mathbf{X} = \mathbf{X}_{(i)}^T\mathbf{X}_{(i)} + \mathbf{x}_i\mathbf{x}_i^T$ rearrange to get $\mathbf{X}_{(i)}^T\mathbf{X}_{(i)} = \mathbf{X}^T\mathbf{X} - \mathbf{x}_i\mathbf{x}_i^T$
- Special Case of Binomial Inverse Theorem or Woodbury Theorem: (Thm B.56 in Christensen)

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

with $\mathbf{A} = \mathbf{X}^T\mathbf{X}$ and $\mathbf{u} = -\mathbf{x}_i$ and $\mathbf{v} = \mathbf{x}_i$

$$(\mathbf{X}_{(i)}^T\mathbf{X}_{(i)})^{-1} = (\mathbf{X}^T\mathbf{X} - \mathbf{x}_i\mathbf{x}_i^T)^{-1} = (\mathbf{X}^T\mathbf{X})^{-1} + \frac{(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i\mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}}{1 - \mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i}$$

- use $\mathbf{X}_i^T\mathbf{Y}_i = \mathbf{X}^T\mathbf{Y} - \mathbf{x}_i y_i$ to get $\hat{\boldsymbol{\beta}}_{(i)}$ and other quantities

External estimate of σ^2

Estimate $\hat{\sigma}^2_{(i)}$ using data with case i deleted

$$\textsf{SSE}_{(i)} = \textsf{SSE} - \frac{e_i^2}{1 - h_{ii}}$$

$$\hat{\sigma}^2_{(i)} = \textsf{MSE}_{(i)} = \frac{\textsf{SSE}_{(i)}}{n - p - 1}$$

- Externally Standardized residuals

$$t_i = \frac{e_{(i)}}{\sqrt{\hat{\sigma}^2_{(i)}/(1 - h_{ii})}} = \frac{y_i - \mathbf{x}_i^T \hat{\boldsymbol{\beta}}_{(i)}}{\sqrt{\hat{\sigma}^2_{(i)}/(1 - h_{ii})}} = r_i \left(\frac{n - p - 1}{n - p - r_i^2} \right)^{1/2}$$

- May still miss extreme points with high leverage, but will pick up unusual y_i's

Externally Studentized Residual

- Externally studentized residuals have a t distribution with $n-p-1$ degrees of freedom:

$$t_i = \frac{e_{(i)}}{\sqrt{\hat{\sigma}^2_{(i)}/(1-h_{ii})}} = \frac{y_i - \mathbf{x}_i^T \hat{\boldsymbol{\beta}}_{(i)}}{\sqrt{\hat{\sigma}^2_{(i)}/(1-h_{ii})}} \sim \mathsf{St}(n-p-1)$$

  under the hypothesis that the ith case is not an "outlier".

- This externally studentized residual statistic is equivalent to the t-statistic for testing that α_i is zero!

(HW)

Multiple Testing

- without prior reason to suspect an outlier, usually look at the maximum of the $|t_i|$'s
- is the $\max |t_i|$ larger than expected under the null of no outliers?
- Need distribution of the max of Student t random variables (simulation?)
- a conservative approach is the Bonferroni Correction: For n tests of size α the probability of falsely labeling at least one case as an outlier is no greater than $n\alpha$; e.g. with 21 cases and $\alpha = 0.05$, the probability is no greater than 1.05!
- adjust $\alpha^* = \alpha/n$ so that the probability of falsely labeling at least one point an outlier is α
- with 21 cases and $\alpha = 0.05$,
  $\alpha/n = .00238$ so use $\alpha^* = 0.0024$ for each test

Influence - Cook's Distance

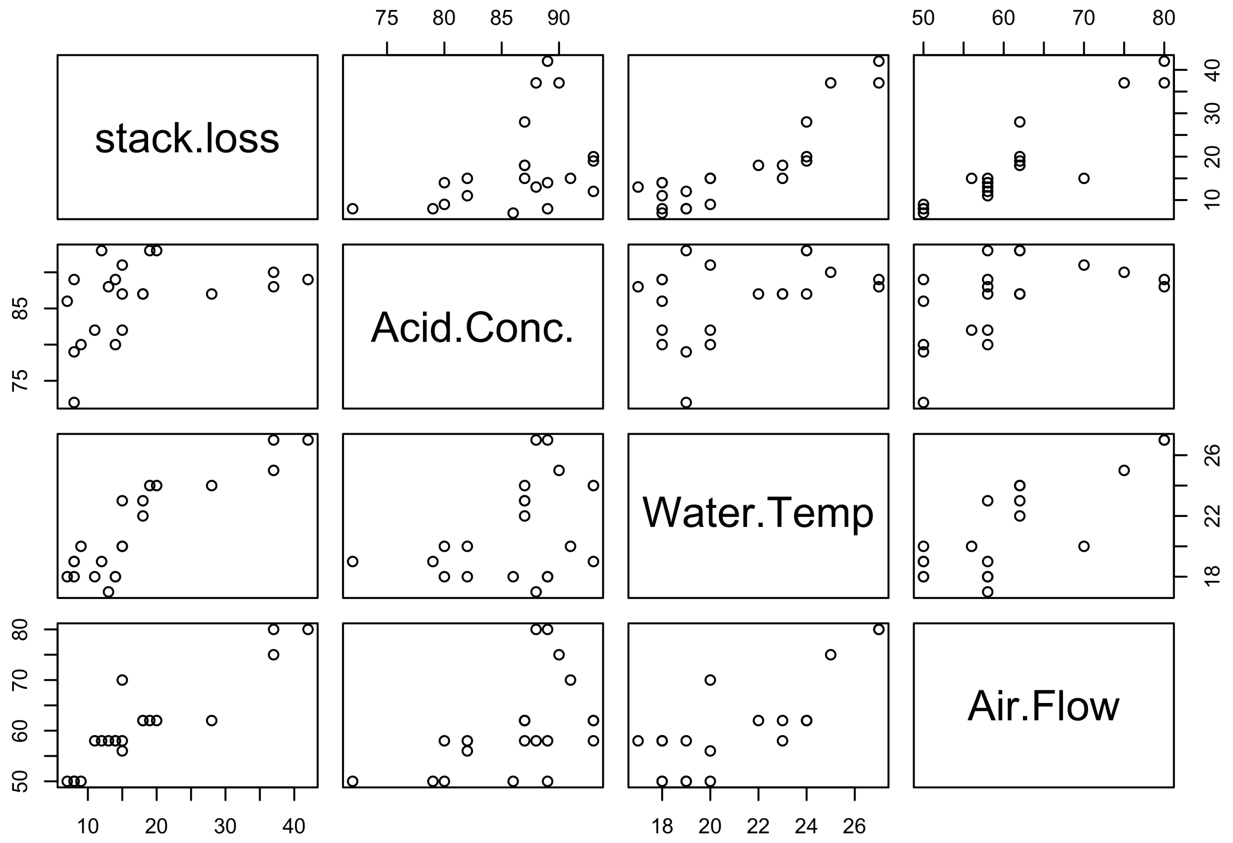
- Cook's Distance measure of how much predictions change with ith case deleted

$$D_i = \frac{\|\hat{\mathbf{Y}}_{(i)} - \hat{\mathbf{Y}}\|^2}{p\hat{\sigma}^2} = \frac{(\hat{\boldsymbol{\beta}}_{(i)} - \hat{\boldsymbol{\beta}})^T \mathbf{X}^T \mathbf{X} (\hat{\boldsymbol{\beta}}_{(i)} - \hat{\boldsymbol{\beta}})}{p\hat{\sigma}^2}$$

$$= \frac{r_i^2}{p} \frac{h_{ii}}{1 - h_{ii}}$$

- Flag cases where $D_i > 1$ or large relative to other cases
- Influential Cases are those with extreme leverage or large r_i^2

Stackloss Data



Case 21

- Leverage 0.285 (compare to $p/n = .19$)
- p-value t_{21} is 0.0042
- Bonferroni adjusted p-value is 0.0024 (not really an outlier?)
- Cooks' Distance $.69$
- Other points? Masking?
- Refit without Case 21 and compare results

Other analyses have suggested that cases (1, 2, 3, 4, 21) are outliers

- look at `MC3.REG` or `BAS` or robust regression

Bayesian Outlier Detection

Chaloner & Brant (1988) "A Bayesian approach to outlier detection and residual analysis"

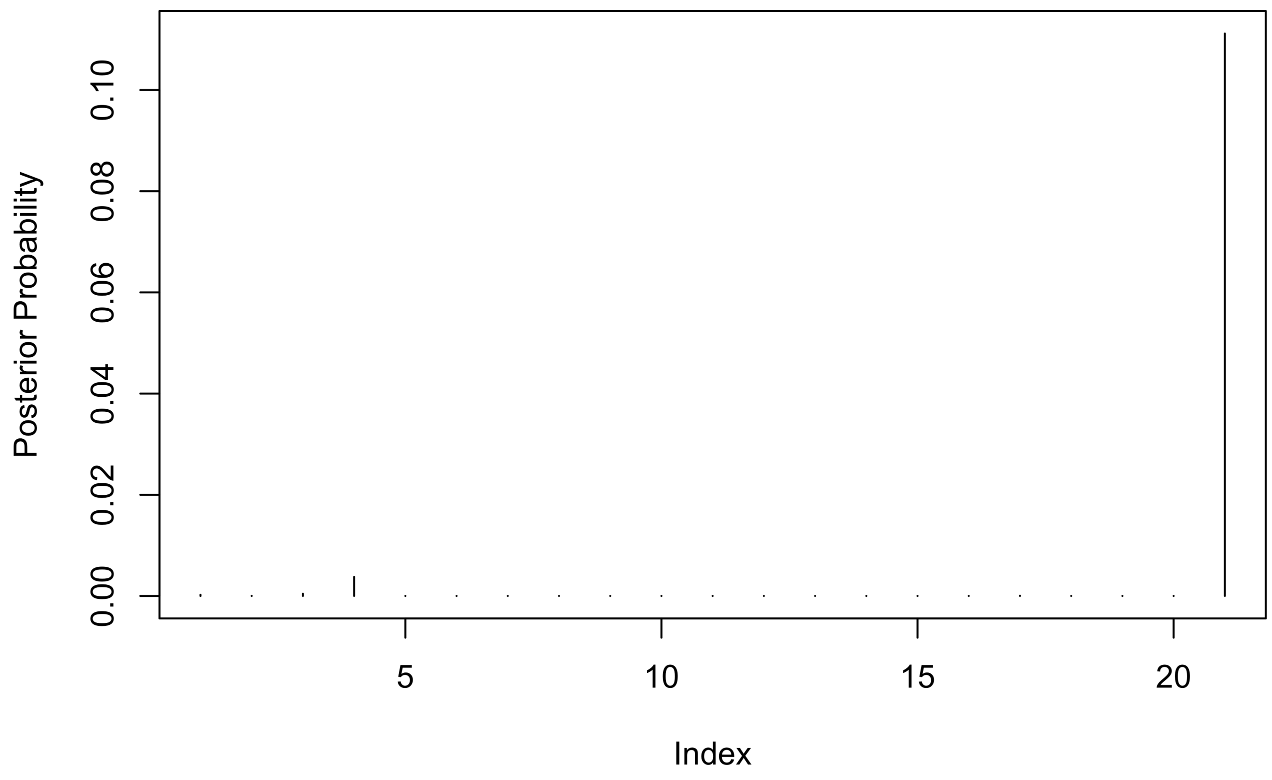
- provides an approach to identify outliers or surprising variables by looking at the probabilty that the *error* for a case is more than k standard deviations above or below zero.

$$P(|e_i| > k\sigma \mid \mathbf{Y})$$

- Cases with a high probability (absolute fixed value of k or relative to a multiplicity correction to determine k) are then investigated.
- find posterior distribution of e_i given the data and model
- Chaloner and Brant use a reference prior for the analysis $p(\boldsymbol{\beta}, \phi) \propto 1/\phi$
- no closed form solution for the probability but can be approximated by MCMC or a one dimensional integral! see `?BAS::Bayes.outlier`

Stackloss Data

```r
library(BAS)
stack.lm <- lm(stack.loss ~ ., data = stackloss)
stack.outliers <- BAS::Bayes.outlier(stack.lm, k = 3)
plot(stack.outliers$prob.outlier,
     type = "h",
     ylab = "Posterior Probability")
```


Posterior Probability
0.00
0.02
0.04
0.06
0.08
0.10
5
10
15
20
Index

Stackloss Data

Adjust prior probability for multiple testing with sample size of 21 and prior probability of no outliers 0.95

```
stack.outliers <- BAS::Bayes.outlier(stack.lm, prior.prob = 0.95)
```

To Remove or Not Remove?

- For suspicious cases, check data sources for errors
- Check that points are not outliers/influential because of wrong mean function or distributional assumptions (transformations)
- Investigate need for transformations (use EDA at several stages)
- Influential cases - report results with and without cases (results may change - are differences meaningful?)
- Outlier test - suggests alternative population for the case(s); if keep in analysis, will inflate $\hat{\sigma}^2$ and interval estimates
- Document how you handle any case deletions - reproducibility!
- If lots of outliers - consider throwing out the model rather than data
- Alternative Model Averaging with Outlier models
- Robust Regression Methods - M-estimation, L-estimation, S-estimation, MM-estimation, etc. or Bayes with heavy tails