Stat GR 5025 Lecture 9

Jingchen Liu

Department of Statistics
Columbia University

Quantification of multicollinearity

$$y, x_1, x_2, \ldots, x_p$$

- With all covariates standardized, we consider

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

- $Var(\hat{\beta}_1) = \sigma^2/(n-1)$
- Consider

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_p x_p + \varepsilon$$

- $Var(\tilde{\beta}) = \sigma^2 (X^\top X)^{-1}$

Quantification of multicollinearity

$$y, x_1, x_2, \ldots, x_p$$

- With all covariates standardized, we consider

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

- $Var(\hat{\beta}_1) = \sigma^2/(n-1)$
- Consider

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_p x_p + \varepsilon$$

- $Var(\tilde{\beta}) = \sigma^2 (X^\top X)^{-1}$

Quantification of multicollinearity

$$y, x_1, x_2, \ldots, x_p$$

- With all covariates standardized, we consider

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

- $Var(\hat{\beta}_1) = \sigma^2/(n-1)$
- Consider

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_p x_p + \varepsilon$$

- $Var(\tilde{\beta}) = \sigma^2 (X^\top X)^{-1}$

Quantification of multicollinearity

$$y, x_1, x_2, \ldots, x_p$$

- With all covariates standardized, we consider

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

- $Var(\hat{\beta}_1) = \sigma^2/(n-1)$
- Consider

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_p x_p + \varepsilon$$

- $Var(\tilde{\beta}) = \sigma^2(X^\top X)^{-1}$

Quantification of multicollinearity

- Variance inflation factor (VIF)

$$VIF(\beta_1) = \frac{Var(\tilde{\beta}_1)}{Var(\hat{\beta}_1)}$$

- A representation

$$VIF(\beta_1) = \frac{1}{1 - R_1^2}$$

where R_1^2 is the coefficient of determination of x_1 on x_2, $x_3, \ldots, x_p$.

Quantification of multicollinearity

- Variance inflation factor (VIF)

$$VIF(\beta_1) = \frac{Var(\tilde{\beta}_1)}{Var(\hat{\beta}_1)}$$

- A representation

$$VIF(\beta_1) = \frac{1}{1 - R_1^2}$$

where R_1^2 is the coefficient of determination of x_1 on x_2, $x_3, \ldots, x_p$.

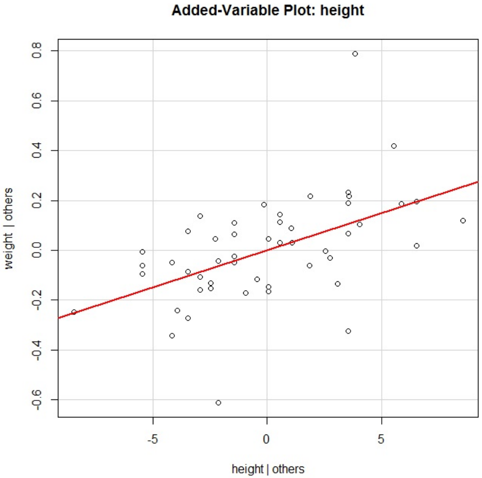
Ridge regression

- The estimator

$$\hat{\beta} = (X^\top X + \Gamma)^{-1} X^\top Y$$

- Discussion

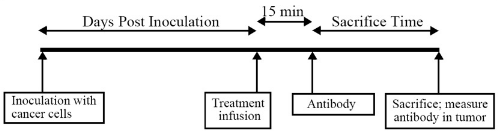
Value-added plot



Outlier detection

Display 11.3 **p. 307**

Time line for blood-brain barrier disruption experiment



Outlier detection

Display 11.4 **p. 308**

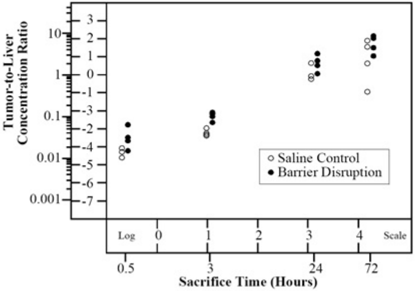
Response variable, design variables, and several covariates for 34 rats in the blood-brain barrier disruption experiment

Case	Response Variable: Brain tumor Count (per gm) / Liver Count (per gm)	Design Variables: Sacrifice Time (hours)	Design Variables: Treatment	Covariates: Days Post Inoculation	Covariates: Sex	Covariates: Initial Weight (grams)	Covariates: Weight Loss (grams)	Covariates: Tumor Weight (10^{-4} grams)
1	41081 / 1456164	0.5	BD	10	F	239	5.9	221
2	44286 / 1602171	0.5	BD	10	F	225	4.0	246
3	102926 / 1601936	0.5	BD	10	F	224	-4.9	61
4	25927 / 1776411	0.5	BD	10	F	184	9.8	168
5	42643 / 1351184	0.5	BD	10	F	250	6.0	164
6	31342 / 1790863	0.5	NS	10	F	196	7.7	260
7	22815 / 1633386	0.5	NS	10	F	200	0.5	27
8	16629 / 1618757	0.5	NS	10	F	273	4.0	308
9	22315 / 1567602	0.5	NS	10	F	216	2.8	93
10	77961 / 1060057	3	BD	10	F	267	2.6	73
11	73178 / 715581	3	BD	10	F	263	1.1	25
12	76167 / 620145	3	BD	10	F	228	0.0	133
13	123730 / 1068423	3	BD	9	F	261	3.4	203
14	25569 / 721436	3	NS	9	F	253	5.9	159
15	33803 / 1019352	3	NS	10	F	234	0.1	264
16	24512 / 667785	3	NS	10	F	238	0.8	34
17	50545 / 961097	3	NS	9	F	230	7.0	146
18	50690 / 1220677	3	NS	10	F	207	1.5	212
19	84616 / 48815	24	BD	10	F	254	3.9	155
20	55153 / 16885	24	BD	10	M	256	-4.7	190
21	48829 / 22395	24	BD	10	M	247	-2.8	101
22	89454 / 83504	24	BD	11	F	198	4.2	214
23	37928 / 20323	24	NS	10	F	237	2.5	224
24	12816 / 15985	24	NS	10	M	293	3.1	151
25	23734 / 25895	24	NS	10	M	288	9.7	285
26	31097 / 33224	24	NS	11	F	236	5.9	380
27	35395 / 4142	72	BD	11	F	251	4.1	39
28	18270 / 2364	72	BD	10	F	223	4.0	153
29	5625 / 1979	72	BD	10	M	298	12.8	164
30	7497 / 1659	72	BD	10	M	260	7.3	364
31	6250 / 928	72	NS	10	M	272	11.0	484
32	11519 / 2423	72	NS	11	F	226	2.2	168
33	3184 / 1608	72	NS	10	M	249	-4.4	191
34	1334 / 3242	72	NS	10	F	240	6.7	159

Outlier detection

Display 11.5 p. 309

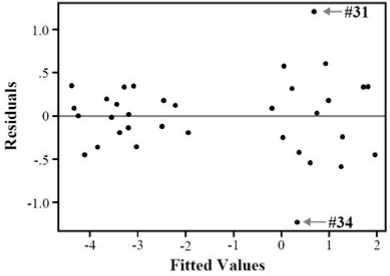
Log-log scatterplot of ratio of antibody concentration in brain tumor to antibody concentration in liver versus sacrifice time, for 17 rats given the barrier disruption infusion and 17 rats given a saline (control) infusion



Outlier detection

Display 11.6 **p. 312**

Scatterplot of residuals versus fitted values from the fit of the logged response on a rich model for explanatory variables; brain barrier data



Deleted residual

$$d_i = y_i - \hat{y}_{i(i)} = \frac{y_i - \hat{y}_i}{1 - h_i} \quad Var(d_i) = \frac{\sigma^2}{1 - h_i}$$

Studentized residual

- Studentized residual

$$StudRes_i = \frac{d_i}{SE(d_i)}$$

- Another representation

$$StudRes_i = \frac{y_i - \hat{y}_i}{SE(y_i - \hat{y}_i)} = \frac{y_i - \hat{y}_i}{\hat{\sigma}\sqrt{1 - h_i}}$$

- About the hat matrix

Studentized residual

- Studentized residual

$$StudRes_i = \frac{d_i}{SE(d_i)}$$

- Another representation

$$StudRes_i = \frac{y_i - \hat{y}_i}{SE(y_i - \hat{y}_i)} = \frac{y_i - \hat{y}_i}{\hat{\sigma}\sqrt{1 - h_i}}$$

- About the hat matrix

Studentized residual

- Studentized residual

$$StudRes_i = \frac{d_i}{SE(d_i)}$$

- Another representation

$$StudRes_i = \frac{y_i - \hat{y}_i}{SE(y_i - \hat{y}_i)} = \frac{y_i - \hat{y}_i}{\hat{\sigma}\sqrt{1 - h_i}}$$

- About the hat matrix

Leverage

- About leverage
- Simple linear model

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum(x_i - \bar{x})^2}$$

- Multiple regression
- Total leverage

Leverage

- About leverage
- Simple linear model

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum(x_i - \bar{x})^2}$$

- Multiple regression
- Total leverage

Leverage

- About leverage
- Simple linear model

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2}$$

- Multiple regression
- Total leverage

Leverage

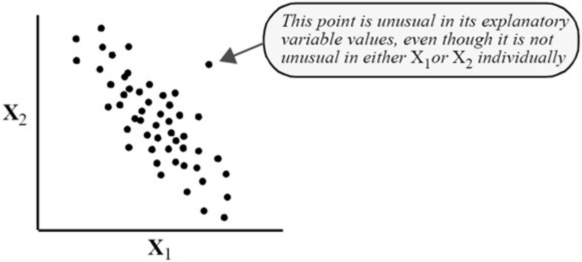
- About leverage
- Simple linear model

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum(x_i - \bar{x})^2}$$

- Multiple regression
- Total leverage

High leverage

An illustration of what is meant by "far from the average" of multiple explanatory variables when they are correlated



Leave-one-out measure

- DIFFITS

$$DIFFITS_i = \frac{\hat{y}_i - \hat{y}_{i(i)}}{\hat{\sigma}_{(i)}\sqrt{h_i}}$$

Leave-one-out measure

- Cook's distance

$$D_i = \frac{\sum_i (\hat{y}_i - \hat{y}_{i(i)})^2}{p\sigma^2}$$

- Another representation

$$D_i = \frac{(y_i - \hat{y}_i)^2}{p\sigma^2}\frac{h_i}{(1-h_i)^2} = \frac{StudRes_i^2}{p}\frac{h_i}{1-h_i}$$

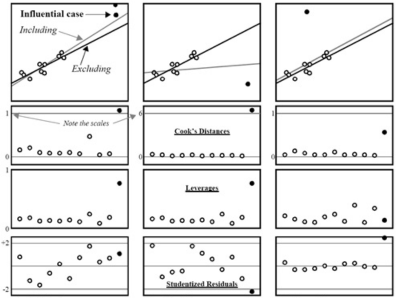
Leave-one-out measure

- DFBETAS

$$DFBETAS_{k(i)} = \frac{\beta_k - \beta_{k(i)}}{\sigma\sqrt{c_k}}$$

Influential points

Three examples of influential cases in simple linear regression. The top row shows regression lines with and without the influential case included. The next three rows show the resulting case influence statistic plots: Cook's distances, leverages, and Studentized residuals. The horizontal axes for the case statistic plots show the case numbers (=11 for the influential case).



A. High leverage and mild departure changes the slope so that the residual is small. Cook's distance identifies the offending case.	B. High leverage and huge departure drastically pulls the line away from all observations. Cook's distance identifies the case.	C. Low leverage does not allow the large departure to alter the slope, so it ends up with a big residual. Cook's distance shows a mild problem.

Influential statitistics

- Studentized residual
- Leverage
- Cook's distance

Model/variable selection

- What is model/variable selection
- Motivation
- Including redundant explanatory variables reduces prediction power
- Large p small n problem

Model/variable selection

- What is model/variable selection
- Motivation
- Including redundant explanatory variables reduces prediction power
- Large p small n problem

Model/variable selection

- What is model/variable selection
- Motivation
- Including redundant explanatory variables reduces prediction power
- Large p small n problem

Model/variable selection

- What is model/variable selection
- Motivation
- Including redundant explanatory variables reduces prediction power
- Large p small n problem

Applications

- Bioinformatics
- Wavelet
- Time series analysis
- Any time you have an alternative model

Applications

- Bioinformatics
- Wavelet
- Time series analysis
- Any time you have an alternative model

Applications

- Bioinformatics
- Wavelet
- Time series analysis
- Any time you have an alternative model

Applications

- Bioinformatics
- Wavelet
- Time series analysis
- Any time you have an alternative model

General questions

- What makes a good model?
  - Small prediction error
  - Large R^2
- Criteria for comparing different models

General questions

- What makes a good model?
  - Small prediction error
  - Large R^2
- Criteria for comparing different models

General questions

- What makes a good model?
  - Small prediction error
  - Large R^2
- Criteria for comparing different models

General questions

- What makes a good model?
  - Small prediction error
  - Large R^2
- Criteria for comparing different models

Some examples

$$H_0 : y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

$$H_1 : y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \varepsilon$$

Some examples

$$H_0 : y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \varepsilon$$

$$H_1 : y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_4 x_4 + \varepsilon$$

Some examples

$$H_0 : y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \boxed{\beta_5 x_5} + \varepsilon$$

$$H_1 : y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \boxed{\beta_3 x_3 + \beta_4 x_4} + \varepsilon$$

Some principles

- What makes a good model?
  - Smaller estimated errors
  - Simpler model/fewer predictors
  - Prediction of *future* observations
- The least squares estimate only considers small fitted errors?

Candidates

- Coefficient of determination, R^2
- Estimated error level, $\hat{\sigma}^2$
- Adjusted R^2

$$\frac{Var(y) - \hat{\sigma}^2}{Var(y)}$$

Algorithmic approach

- Forward selection
- Backward deletion
- Stepwise regression

Forward selection

- Consider variables that are not in the current model, compute the extra-sum-of-squares by adding each variable.
- If the largest extra-sum-of-squares is greater than some value (e.g., 4), then add that variable in; otherwise stop.

Backward deletion

- Consider variables that are in the current model, compute the extra-sum-of-squares by removing each variable.
- If the smallest extra-sum-of-squares is less than some value (e.g., 4), then remove that variable; otherwise stop.

Stepwise regression

- Do one step forward selection and backward deletion alternatively

Pros and cons

- Easy to implement
- Less computation
- In consistency

Likelihood-based criteria

- Akaike information criterion (AIC)

$$n \log(\hat{\sigma}^2) + 2p.$$

Derive AIC.

- Bayesian information criterion

$$n \log(\hat{\sigma}^2) + p \log(n)$$

General form

$$x_1, \ldots, x_n \sim f(x|\theta)$$

- Akaike information criterion (AIC)

$$-2\log(L(\hat{\theta})) + 2p$$

- Bayesian information criterion

$$-2\log(L(\hat{\theta})) + p\log(n)$$

General form

- Likelihood

$$L(\theta; x_1, ..., x_n)$$

- Maximum likelihood estimator
- Derivation of AIC

Mallows' C_p

- Let $\mu_i = E(y|x_i)$.
- Mean squared error

$$E[(\hat{y}_i - \mu_i)^2|x_i] = E^2(\hat{y}_i - \mu_i|x_i) + Var(\hat{y}_i - \mu_i|x_i)$$

- Total mean squared error

$$\sum_{i=1}^{n} E[(\hat{y}_i - \mu_i)^2|x_i] = \sum_{i=1}^{n} E^2(\hat{y}_i - \mu_i|x_i) + \sum_{i=1}^{n} Var(\hat{y}_i - \mu_i|x_i)$$

Mallows' C_p

- Let $\mu_i = E(y|x_i)$.
- Mean squared error

$$E[(\hat{y}_i - \mu_i)^2|x_i] = E^2(\hat{y}_i - \mu_i|x_i) + Var(\hat{y}_i - \mu_i|x_i)$$

- Total mean squared error

$$\sum_{i=1}^{n} E[(\hat{y}_i - \mu_i)^2|x_i] = \sum_{i=1}^{n} E^2(\hat{y}_i - \mu_i|x_i) + \sum_{i=1}^{n} Var(\hat{y}_i - \mu_i|x_i)$$

Mallows' C_p

- Let $\mu_i = E(y|x_i)$.
- Mean squared error

$$E[(\hat{y}_i - \mu_i)^2|x_i] = E^2(\hat{y}_i - \mu_i|x_i) + Var(\hat{y}_i - \mu_i|x_i)$$

- Total mean squared error

$$\sum_{i=1}^{n} E[(\hat{y}_i - \mu_i)^2|x_i] = \sum_{i=1}^{n} E^2(\hat{y}_i - \mu_i|x_i) + \sum_{i=1}^{n} Var(\hat{y}_i - \mu_i|x_i)$$

Mallows' C_p

$$C_p = \frac{SSE}{\hat{\sigma}_f^2} - (n - 2p) = p + (n - p)\frac{\hat{\sigma}^2 - \hat{\sigma}_f^2}{\hat{\sigma}_f^2}$$