## Purdue-NCKU program

# Lecture 8 <br> Multiple Linear Regression 

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## The Data and Model

- Still have single response variable $Y$
- Now have multiple explanatory variables
- Examples:
- Blood Pressure vs Age, Weight, Diet, Fitness Level
- Traffic Count vs Time, Location, Population, Month
- Goal: There is a total amount of variation in $Y$ (SSTO). We want to explain as much of this variation as possible using a linear model and our explanatory variables

$$
Y_{i}=\beta_{0}+\beta_{1} X_{i 1}+\cdots+\beta_{p-1} X_{i, p-1}+\varepsilon_{i}
$$

- Have $p$ - 1 predictors $\longrightarrow p$ coefficients


## General Linear Model

However, it can be much more flexible than just using the original response and explanatory variables in your data set

- Polynomial regression:

$$
\begin{aligned}
Y_{i} & =\beta_{0}+\beta_{1} X_{i}+\beta_{2} X_{i}^{2}+\varepsilon_{i} \\
& :=\beta_{0}+\beta_{1} X_{i 1}+\beta_{2} X_{i 2}+\varepsilon_{i}
\end{aligned}
$$

- cross product term:

$$
\begin{aligned}
Y_{i} & =\beta_{0}+\beta_{1} X_{i 1}+\beta_{2} X_{i 2}+\beta_{3} X_{i 2} * X_{i 1}+\varepsilon_{i} \\
& :=\beta_{0}+\beta_{1} X_{i 1}+\beta_{2} X_{i 2}+\beta_{3} X_{i 3}+\varepsilon_{i}
\end{aligned}
$$

- Transformed response:

$$
\log \left(Y_{i}\right)=\beta_{0}+\beta_{1} X_{i 1}+\beta_{2} X_{i 2}+\varepsilon_{i}
$$

- Factor analysis is also a multiple linear regression

Still linear models (of $\beta$ 's), while the meaning of $\beta$ is different (will discussed later)

## General Linear Regression In Matrix Terms

- After transformation and re-organization, a linear model ("linear" w.r.t. unknown coefficient, not to actual predictors) is obtained

$$
Y_{i}=\beta_{0}+\beta_{1} X_{i 1}+\cdots+\beta_{p-1} X_{i, p-1}+\varepsilon_{i}
$$

- As an array

$$
\left[\begin{array}{c}
Y_{1} \\
Y_{2} \\
\vdots \\
Y_{n}
\end{array}\right]=\left[\begin{array}{ccccc}
1 & X_{11} & X_{12} & \cdots & X_{1}{ }_{p-1} \\
1 & X_{21} & X_{22} & \cdots & X_{2}{ }_{p-1} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
1 & X_{n 1} & X_{n 2} & \cdots & X_{n} \\
&
\end{array}\right]\left[\begin{array}{c}
\beta_{0} \\
\beta_{1} \\
\beta_{2} \\
\vdots \\
\beta_{p-1}
\end{array}\right]+\left[\begin{array}{c}
\varepsilon_{1} \\
\varepsilon_{2} \\
\vdots \\
\varepsilon_{n}
\end{array}\right]
$$

- In matrix notation

$$
\mathbf{Y}=\mathbf{X} \boldsymbol{\beta}+\varepsilon
$$

- Distributional assumptions:

$$
\varepsilon \sim N\left(0, \sigma^{2} I\right) \longrightarrow \mathbf{Y} \sim N\left(\mathbf{X} \boldsymbol{\beta}, \sigma^{2} I\right)
$$

## Estimation, Fitted value and Residuals

- Least squares estimates $b=\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{Y}$
- Fitted values: $\hat{\mathbf{Y}}=\mathbf{X}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{Y}=\mathbf{H Y}$ define a (hyper)plane.
- Residuals: $\mathrm{e}=\mathbf{Y}-\hat{\mathbf{Y}}=(\mathbf{I}-\mathbf{H}) \mathbf{Y}$
- Expected value $E(\mathbf{e})=0$
- Covariance Matrix

$$
\begin{aligned}
\sigma^{2}(\mathbf{e}) & =\sigma^{2}(\mathbf{I}-\mathbf{H})(\mathbf{I}-\mathbf{H})^{\prime} \\
& =\sigma^{2}(\mathbf{I}-\mathbf{H})
\end{aligned}
$$

$-\operatorname{Var}\left(e_{i}\right)=\sigma^{2}\left(1-h_{i i}\right)$ where $h_{i i}=\mathbf{X}_{i}^{\prime}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}_{i}$

- Residuals are usually correlated, i.e., $\operatorname{cov}\left(e_{i}, e_{j}\right)=-\sigma^{2} h_{i j}, i \neq j$
- Will use this information for diagnose


## Estimation of $\sigma^{2}$

- Similar approach as before
- Estimate it from e, since e has nothing to do with $\beta_{i}$ 's.
- Now $p$ model parameters

$$
\begin{aligned}
s^{2} & =\frac{\mathbf{e}^{\prime} \mathbf{e}}{n-p} \\
& =\frac{(\mathbf{Y}-\mathbf{X b})^{\prime}(\mathbf{Y}-\mathbf{X b})}{n-p} \\
& =\frac{\mathrm{SSE}}{n-p} \\
& =\mathrm{MSE}
\end{aligned}
$$

- Specifically, SSE $\sim \sigma^{2} \chi_{\text {rank }}^{2}$ of ( $\mathbf{I}-\mathbf{H}$ )


## ANOVA TABLE

| Source of <br> Variation | df | SS | MS | F Value |
| :--- | :---: | :---: | :---: | :---: |
| Regression <br> (Model) | $p-1$ | SSR | $\mathrm{MSR}=\mathrm{SSR} /(p-1)$ | $\mathrm{MSR} / \mathrm{MSE}$ |
| Error | $n-p$ | SSE | $\mathrm{MSE}=\mathrm{SSE} /(n-p)$ |  |

Total $\quad n-1$ SSTO

- F Test: Tests if the predictors collectively help explain the variation in $Y$
$-H_{0}: \beta_{1}=\beta_{2}=\ldots=\beta_{p-1}=0$
- $H_{a}$ : at least one $\beta_{k} \neq 0,1 \leq k \leq p-1$
$-F^{*}=\frac{S S R /(p-1)}{S S E /(n-p)} \stackrel{H_{0}}{\sim} F(p-1, n-p)$
- Reject $H_{0}$ if $F^{*}>F(1-\alpha, p-1, n-p)$
- No conclusions possible regarding individual predictors


## Testing Individual Predictor

- Have already shown that $\mathbf{b} \sim N\left(\boldsymbol{\beta}, \sigma^{2}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1}\right)$
- This implies $b_{k} \sim N\left(\beta_{k}, \sigma^{2}\left(b_{k}\right)\right)$
- Perform $t$ test
$-H_{0}: \beta_{k}=\beta_{k}^{0}$ vs $H_{a}: \beta_{k} \neq \beta_{k}^{0}$
$-t^{*}=\frac{b_{k}-\beta_{k}^{0}}{s\left(b_{k}\right)} \sim t_{n-p}$ under $H_{0}$
- P-value $=\operatorname{Pr}\left(\left|t_{n-p}\right| \geq t^{*}\right)$
- Reject $H_{0}$ if $\left|t^{*}\right|>t(1-\alpha / 2, n-p)$ or P-value $<\alpha$
- Confidence interval for $\beta_{k}$

$$
-b_{k} \pm t(1-\alpha / 2, n-p) s\left\{b_{k}\right\}
$$

## Estimation of Mean Response $E\left(Y_{h}\right)$

- interested in making predictions for a new observation, represented by a $p$ dimensional vector $\mathbf{X}_{h}$
- Can show $\widehat{Y}_{h} \sim N\left(\mathbf{X}_{h}^{\prime} \boldsymbol{\beta}, \sigma^{2} \mathbf{X}_{h}^{\prime}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}_{h}\right)$
- standard error $s\left\{\widehat{Y}_{h}\right\}=\sqrt{\mathrm{MSEX}_{h}^{\prime}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}_{h}}$
- Individual CI for $\mathbf{X}_{h}$
- $\widehat{Y}_{h} \pm t(1-\alpha / 2, n-p) s\left\{\widehat{Y}_{h}\right\}$
- Bonferroni CI for $g$ vectors $\mathbf{X}_{h}$
$-\widehat{Y}_{h} \pm t(1-\alpha /(2 g), n-p) s\left\{\widehat{Y}_{h}\right\}$
- Working-Hotelling confidence band for the whole regression line
$-\widehat{Y}_{h} \pm \sqrt{p F(1-\alpha, p, n-p)} s\left\{\hat{Y}_{h}\right\}$


## Predict New Observation

- $Y_{h(n e w)}=E\left(Y_{h}\right)+\varepsilon$

$$
\begin{aligned}
& -\widehat{Y}_{h}+\varepsilon \sim N\left(\mathbf{X}_{h}^{\prime} \boldsymbol{\beta}, \sigma^{2}\left(1+\mathbf{X}_{h}^{\prime}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}_{h}\right)\right) \\
& -s^{2}(\text { pred })=s^{2}\left(\widehat{Y}_{h}\right)+\mathrm{MSE}
\end{aligned}
$$

- Individual CI of $Y_{h(n e w)}$

$$
-\hat{Y}_{h} \pm t(1-\alpha / 2, n-p) s\{p r e d\}
$$

- Bonferroni CI for $g$ vectors $\mathbf{X}_{h}$

$$
-\widehat{Y}_{h} \pm t(1-\alpha /(2 g), n-p) s\{p r e d\}
$$

## General Linear Test

- Comparison of a full model and reduced model that involves a subset of full model predictors (i.e., hierarchical structure)
- Involves a comparison of unexplained SS
- Consider a full model with $k$ predictors (or $k$ mean parameters) and reduced model with $l$ predictors ( $l<k$ )
- One can prove that $\operatorname{SSE}(\mathrm{R})-\operatorname{SSE}(\mathrm{F}) \geq 0$.
- Can show that under null hypothesis
$F^{\star}=\frac{(\operatorname{SSE}(\mathrm{R})-\operatorname{SSE}(\mathrm{F})) /((n-1-l)-(n-k-1))}{\operatorname{SSE}(\mathrm{F}) /(n-k-1)} \sim F_{k-l, n-k-1}$ distribution
- Degrees of freedom for $F^{*}$ are the number of extra variables and the error degrees of freedom for the full model


## Example

- Testing the null hypothesis that the regression coefficients for the extra variables are all zero.
- $H_{0}: \beta_{k}=0$ vs $H_{a}: \beta_{k} \neq 0$
- Full Model :

$$
Y_{i}=\beta_{0}+\sum_{j=1}^{p-1} \beta_{j} X_{j i}+\varepsilon_{i}
$$

- Reduced Model :

$$
Y_{i}=\beta_{0}+\sum_{j=1}^{k-1} \beta_{j} X_{j i}+\sum_{j=k+1}^{p-1} \beta_{j} X_{j i}+\varepsilon_{i}
$$

$-F^{\star}=\frac{(\operatorname{SSE}(\mathrm{R})-\operatorname{SSE}(\mathrm{F})) / 1}{\operatorname{SSE}(\mathrm{~F}) /(n-p)}$

- Reject $H_{0}$ if $F^{*}>F(1-\alpha, 1, n-p)$
- Can show that $F^{*}=\left(t^{*}\right)^{2}$, i.e., equivalent to the $t$ test


## Extra SS and Notation

- Consider $H_{0}: X_{1}, X_{3}$ vs $H_{a}: X_{1}, X_{2}, X_{3}, X_{4}$
- Null can also be written $H_{0}: \beta_{2}=\beta_{4}=0$
- Write $\operatorname{SSE}(F)$ and $\operatorname{SSE}(\mathrm{R})$ as $\operatorname{SSE}\left(X_{1}, X_{2}, X_{3}, X_{4}\right)$ and $\operatorname{SSE}\left(X_{1}, X_{3}\right)$ respectively
- Difference in SSE's is the extra SS

$$
\operatorname{SSE}\left(X_{2}, X_{4} \mid X_{1}, X_{3}\right)=\operatorname{SSE}\left(X_{1}, X_{3}\right)-\operatorname{SSE}\left(X_{1}, X_{2}, X_{3}, X_{4}\right)
$$

- Recall SSM can also be used

$$
\begin{aligned}
\operatorname{SSM}\left(X_{2}, X_{4} \mid X_{1}, X_{3}\right) & =\operatorname{SSM}\left(X_{1}, X_{2}, X_{3}, X_{4}\right)-\operatorname{SSM}\left(X_{1}, X_{3}\right) \Longrightarrow \\
\operatorname{SSM}\left(X_{1}, X_{2}, X_{3}, X_{4}\right) & =\operatorname{SSM}\left(X_{1}, X_{3}\right)+\operatorname{SSM}\left(X_{2}, X_{4} \mid X_{1}, X_{3}\right)
\end{aligned}
$$

- Can rewrite $F$ test as

$$
F^{\star}=\frac{\operatorname{SSE}\left(X_{2}, X_{4} \mid X_{1}, X_{3}\right) /(4-2)}{\operatorname{SSE}\left(X_{1}, X_{2}, X_{3}, X_{4}\right) /(n-5)}
$$

- If it is possible that neither $H_{0}$ nor $H_{1}$ is correct, large p-value doesn't necessary provide evidence for $H_{0}$, but still serves as an evaluation tool for the usefulness of the additional predictors in $H_{1}$.


## Type I SS and Type II SS

- Type I and Type II are very different
- Type I is sequential, so it depends on model statement
- Type II is conditional on all others, so it does not depend on model statement
- For example, model y = x1 x2 x3 yields

| Type I | Type II |
| :--- | :--- |
| $\operatorname{SSM}\left(X_{1}\right)$ | $\operatorname{SSM}\left(X_{1} \mid X_{2}, X_{3}\right)$ |
| $\operatorname{SSM}\left(X_{2} \mid X_{1}\right)$ | $\operatorname{SSM}\left(X_{2} \mid X_{1}, X_{3}\right)$ |
| $\operatorname{SSM}\left(X_{3} \mid X_{1}, X_{2}\right)$ | $\operatorname{SSM}\left(X_{3} \mid X_{1}, X_{2}\right)$ |

- Could variables be explaining same SS and "canceling" each other out, such that we need to cautions about testing results?
- A case study

- Set of three variables helpful in predicting body fat ( $P<0.0001$ )
- None of the individual parameters is significant
- Addition of each predictor to a model containing the other two is not helpful
- More than $90 \%$ of Type I SS of skinfold can also be explained by thigh and midarm


## Multicollinearity

- Numerical analysis problem is that the matrix $\mathbf{X}^{\prime} \mathbf{X}$ is almost singular (linear dependent columns)
- Makes it difficult to take the inverse
- Generally handled with current algorithms
- Statistical problem: too much correlation among predictors
- The coefficient estimation lacks interpretability.
- Difficult to determine regression coefficients $\longrightarrow$ Increased standard error
- May not affect prediction accuracy if the testing samples follow similar multicollinear correlation.
- Want to refine model to remove redundancy in the predictors
- Investigate the model via general linear tests: fat=skinfold

| Analysis of Variance |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Source |  | Sum of Mean |  |  |  | F Value Pr > F |  |
|  |  | DF | Squares |  | uare |  |  |
| Model |  | 1 | 352.26980 | 352. | 6980 | 44.30 | <. 0001 |
| Error |  | 18 | 143.11970 | 7.9 | 5109 |  |  |
| Corrected | Total | 19 | 495.38950 |  |  |  |  |
|  |  |  | rameter Est | imates |  |  |  |
|  |  | Para | eter Stand | dard |  |  |  |
| Variable | DF | Esti | ate E | ror t | Value | Pr | $\|t\|$ |
| Intercept | 1 | -1. | 610 3.3 | 923 | -0.45 |  | 6576 |
| skinfold | 1 | 0.8 | $719 \quad 0.12$ | 878 | 6.66 |  | 0001 |

- Skinfold now helpful. Note the change in coefficient estimate and standard error compared to the full model.


## Residuals for Diagnostics

- $\mathrm{e}=\mathrm{Y}-\hat{\mathrm{Y}}=(\mathbf{I}-\mathbf{H}) \mathbf{Y}$
- I - H symmetric and idempotent
- Expected value $E(\mathbf{e})=0$
- Covariance matrix

$$
\begin{aligned}
\sigma^{2}(\mathbf{e}) & =\sigma^{2}(\mathbf{I}-\mathbf{H})(\mathbf{I}-\mathbf{H})^{\prime} \\
& =\sigma^{2}(\mathbf{I}-\mathbf{H})
\end{aligned}
$$

$-\operatorname{Var}\left(e_{i}\right)=\sigma^{2} \cdot\left(1-h_{i i}\right)$ where $h_{i i}=\mathbf{X}_{i}^{\prime}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}_{i}$
$-\operatorname{Cov}\left(e_{i}, e_{j}\right)=\sigma^{2} \cdot\left(0-h_{i j}\right)=-\sigma^{2} h_{i j}$

- Estimated variance and covariance
$-\widehat{\operatorname{Var}}\left(e_{i}\right)=M S E \cdot\left(1-h_{i i}\right)$
$-\widehat{\operatorname{Cov}}\left(e_{i}, e_{j}\right)=-M S E \cdot h_{i j}$


## Residuals

- Ordinary residual

$$
e_{i}=Y_{i}-\widehat{Y}_{i} \rightarrow \mathbf{e} \sim \operatorname{MVN}\left(\mathbf{0},(\mathbf{I}-\mathbf{H}) \sigma^{2}\right)
$$

- residuals do not have the same variance, but depend on $\mathbf{X}_{i}$
- Semi-studentized residual

$$
r_{i}=\frac{e_{i}}{\sqrt{\mathrm{MSE}}}
$$

- denominator is not an estimate of SD of $e_{i}$
- (Internally) Studentized Residual

$$
r_{i}=\frac{e_{i}}{\sqrt{\operatorname{MSE}\left(1-h_{i i}\right)}}
$$

- denominator is the estimate of SD of $e_{i}$
- "Studentized" residual doesn't follow the student $t$ distribution (but a $\tau$ distribution)
- Outlier may not have a outstanding studentized residual


## Deleted Residual

- Deleted residual (a refinement of residual)

$$
d_{i}=Y_{i}-\widehat{Y}_{i(i)}=\frac{e_{i}}{1-h_{i i}}
$$

- $\left(\mathbf{X}_{i}, Y_{i}\right)$ was not used to fit the model
- can calculate $d_{i}$ in a single model fit
- Standard deviation of deleted residuals

$$
\begin{aligned}
s^{2}\left\{d_{i}\right\} & =M S E_{(i)} \cdot\left(1+\mathbf{X}_{i}^{\prime}\left(\mathbf{X}_{(i)}^{\prime} \mathbf{X}_{(i)}\right)^{-1} \mathbf{X}_{i}\right) \\
& =\frac{M S E_{(i)}}{1-h_{i i}}
\end{aligned}
$$

- Studentized deleted residual (externally studentized residual)

$$
\begin{aligned}
t_{i} & =\frac{d_{i}}{s\left\{d_{i}\right\}}=\frac{e_{i}}{1-h_{i i}} \cdot \sqrt{\frac{1-h_{i i}}{M S E_{(i)}}} \\
& =\frac{e_{i}}{\sqrt{M S E_{(i)}\left(1-h_{i i}\right)}}
\end{aligned}
$$

## Studentized Deleted Residuals

- If there is only one outlier, its studentized deleted residual will be outstanding
- Useful for identifying outlying $Y$ observation
- Test $H_{i 0}: E\left[Y_{i}\right]=X_{i} \beta$ vs $H_{i a}: E\left[Y_{i}\right] \neq X_{i} \beta$
- If there are no outlying observations,

$$
t_{i} \sim t_{n-1-p}
$$

- can compare $t_{i}$ to this reference distribution
- adjust for $n$ tests using Bonferroni
- an outlier has $\left|t_{i}\right|>t_{1-\alpha /(2 n)}(n-1-p)$
- $t_{i}$ are not independent


## Identifying Outlying X: Hat Matrix Diagonals

- Diagonals $0 \leq h_{i i} \leq 1$ and sum to $p$
- Also known as the leverage of $i$ th case
- Is a measure of distance between the $X$ value and the mean of the $X$ values for all $n$ cases ( $\bar{X}_{1}, \bar{X}_{2}, \ldots, \bar{X}_{p-1}$ )
- Since $\hat{\mathbf{Y}}=\mathbf{H Y}$

$$
\widehat{Y}_{i}=h_{i 1} Y_{1}+h_{i 2} Y_{2}+\ldots+h_{i n} Y_{n}
$$

- Thus $h_{i i}$ is a measure of how much $Y_{i}$ is contributing to the prediction of $\hat{Y}_{i}$


## Hat Matrix Diagonals

- Residual

$$
\begin{aligned}
\mathbf{e} & =(\mathbf{I}-\mathbf{H}) \mathbf{Y} \\
\operatorname{Var}(\mathbf{e}) & =(\mathbf{I}-\mathbf{H}) \sigma^{2} \\
\operatorname{Var}\left(e_{i}\right) & =\left(1-h_{i i}\right) \sigma^{2}
\end{aligned}
$$

- Large $h_{i i}$ means small residual variance
- $\widehat{Y}_{i}$ will be close to $Y_{i}$ (i.e., model is forced to fit this observation closely)
- Observations with large $h_{i i}$ considered influential
- large $h_{i i}$ if it is more than double of the average value, i.e., $h_{i i}>2 p / n$
- Can compute $\mathbf{X}_{\text {new }}^{\prime}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}_{\text {new }}$ to check for hidden extrapolation


## Identifying Influential Cases

## Cook's Distance

- Measures influence of a case on the prediction of all $\hat{Y}_{i}$ 's
- Standardized version of sum of squared differences between fitted values with and without case $i$

$$
D_{i}=\frac{\sum_{j=1}^{n}\left(\hat{Y}_{j}-\hat{Y}_{j(i)}\right)^{2}}{p \cdot \mathrm{MSE}}=\frac{\left(\mathbf{b}_{(i)}-\mathbf{b}\right)^{\prime}\left(\mathbf{X}^{\prime} \mathbf{X}\right)\left(\mathbf{b}_{(i)}-\mathbf{b}\right)}{p \cdot \mathrm{MSE}}
$$

- can be obtained in a single fit

$$
D_{i}=\frac{e_{i}^{2} h_{i i}}{p \operatorname{MSE}\left(1-h_{i i}\right)^{2}}
$$

- Compare with $F(p, n-p)$
- Concern if $D_{i}$ is above the $50 \%$-tile of $F(p, n-p)$


## Multicollinearity Diagnostics: VIF

- Use Variance Inflation Factor (VIF)
- $\mathrm{VIF}_{k}$ is the the $k$ th diagonal element of $r_{X X}^{-1}$ (inverse of sample correlation matrix)

$$
\mathrm{VIF}_{k}=\left(r_{X X}^{-1}\right)_{k k}=\frac{1}{1-R_{k}^{2}}
$$

- where $R_{k}^{2}$ is the coefficient of multiple determination of $X_{k}$ regressed versus all other $p-2$ variables.
- In standardized regression (all $X$ columns are standardized)

$$
\begin{aligned}
\operatorname{Var}\left(\mathbf{b}^{*}\right) & =\left(\sigma^{*}\right)^{2} \mathbf{r}_{X^{\prime} X}^{-1} \\
\operatorname{Var}\left(\mathbf{b}_{k}^{*}\right) & =\left(\sigma^{*}\right)^{2}\left(r_{X X}^{-1}\right)_{k k}=\left(\sigma^{*}\right)^{2} \operatorname{VIF}_{k}
\end{aligned}
$$

- VIF of 10 or more suggests strong multicollinearity
- Also compare mean VIF to 1


## Weighted Least Squares

Downweight influential observations

- The weighted least squares method minimizes

$$
Q_{w}=(\mathbf{Y}-\mathbf{X} \boldsymbol{\beta})^{\prime} \mathbf{W}(\mathbf{Y}-\mathbf{X} \boldsymbol{\beta})
$$

- where $\mathbf{W}=\operatorname{diag}\left\{w_{1}, \cdots, w_{n}\right\}$,
- By taking a derivative of $Q_{w}$, obtain normal equations:

$$
\left(\mathbf{X}^{\prime} \mathbf{W X}\right) \mathbf{b}=\mathbf{X}^{\prime} \mathbf{W} \mathbf{Y}
$$

- Solution of the normal equations:

$$
b=\left(\mathbf{X}^{\prime} \mathbf{W} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{W} \mathbf{Y}
$$

- Can also be viewed as solution for unequal variance scenario


## Unequal Error Variances

- Consider $\mathbf{Y}=\mathbf{X} \boldsymbol{\beta}+\varepsilon$ where $\boldsymbol{\sigma}^{2}(\varepsilon)=\mathbf{W}^{-1}$
- Potentially correlated errors and unequal variances
- Special case: $\mathbf{W}=\operatorname{diag}\left\{w_{1}, w_{2}, \cdots, w_{n}\right\}$
- Heterogeneous variance or heteroscedasticity
- Homogeneous variance or homoscedasticity if $w_{1}=w_{2}=$ $\cdots=w_{n}=1 / \sigma^{2}$
- Least square estimation still yields unbiased estimation, but is no longer optimal, and gives wrong uncertainty quantification
- Consider a transformation based on a known W

$$
\begin{aligned}
\mathbf{W}^{1 / 2} \mathbf{Y} & =\mathbf{W}^{1 / 2} \mathbf{X} \boldsymbol{\beta}+\mathbf{W}^{1 / 2} \varepsilon \\
& \downarrow \\
\mathbf{Y}_{w} & =\mathbf{X}_{w} \boldsymbol{\beta}+\varepsilon_{w}
\end{aligned}
$$

- Can show $\mathrm{E}\left(\varepsilon_{w}\right)=0$ and $\sigma^{2}\left(\varepsilon_{w}\right)=\mathbf{I}$


## Connection

- Least square problem for $\mathbf{Y}_{w}, \mathbf{X}_{w}$

$$
Q_{w}=\left(\mathbf{Y}_{w}-\mathbf{X}_{w} \boldsymbol{\beta}\right)^{\prime}\left(\mathbf{Y}_{w}-\mathbf{X}_{w} \boldsymbol{\beta}\right)=(\mathbf{Y}-\mathbf{X} \boldsymbol{\beta})^{\prime} \mathbf{W}(\mathbf{Y}-\mathbf{X} \boldsymbol{\beta})
$$

- Must determine optimal weights
- Optimal weights $\propto 1 /$ variance
- Methods to determine weights, if no prior information of variance
- Find relationship between the absolute residual and another variable and use this as a model for the standard deviation
- Instead of the absolute residual, use the squared residual and find function for the variance
- Use grouped data or approximately grouped data to estimate the variance


## Ridge Regression as Multicollinearity Remedy

- Modification of least squares that overcomes multicollinearity problem
- Recall least squares suffers because ( $\mathbf{X}^{\prime} \mathbf{X}$ ) is almost singular thereby resulting in highly unstable parameter estimates
- Ridge regression results in biased but more stable estimates
- After standardizing data, we consider the correlation transformation so the normal equations are given by $\mathbf{r}_{X X} \mathbf{b}=\mathbf{r}_{Y X}$. Since $\mathbf{r}_{X X}$ difficult to invert, we add a bias constant, $c$.

$$
\mathbf{b}^{R}=\left(\mathbf{r}_{X X}+c \mathbf{I}\right)^{-1} \mathbf{r}_{Y X}
$$

We then tranform it back to coefficient estimators for the orignal data.

## Choice of $c$

- Key to approach is choice of $c$
- Common to use the ridge trace and VIF's
- Ridge trace: simultaneous plot of $p-1$ parameter estimates for different values of $c \geq 0$. Curves may fluctuate widely when $c$ close to zero but eventually stabilize and slowly converge to 0.
- VIF's tend to fall quickly as $c$ moves away from zero and then change only moderately after that
- Choose $c$ where things tend to "stabilize"



## Chapter Review

- Multiple linear regression
- Estimation and inferences
- Diagnose and Remedy

