# STA 5820 Chapter 3 Linear Regression

Kazuhiko Shinki

Wayne State University

### **Overview:**

Most of the essential features of linear model have already been discussed in (i) Chapters 6 and 11 in STA 5030 and (ii) Chapter 2 of this course. In this chapter, we will discuss

- (a) '1m' function's outputs which have not been discussed.
- (b) how to check assumption of a linear model, and how to deal with violation on assumptions.
- (c) how to handle qualitative (categorical) predictors.
  - testing categorical predictors
  - handling ordered predictors

```
> Dad <- read.table("Advertising.csv".sep=".".header=T)</pre>
> attach(Dad)
> LMB <- lm(sales ~ TV + I(TV^2) + radio)</pre>
> summarv(LMB)
Residuals:
   Min
        10 Median 30 Max
-7.3860 -0.8822 -0.0498 0.9613 3.5725
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.288e+00 3.588e-01 3.588 0.000421 ***
    7.844e-02 4.985e-03 15.736 < 2e-16 ***
TV
I(TV<sup>2</sup>) -1.136e-04 1.677e-05 -6.775 1.42e-10 ***
radio 1.930e-01 7.293e-03 26.465 < 2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 1.517 on 196 degrees of freedom
Multiple R-squared: 0.9167, Adjusted R-squared: 0.9154
F-statistic: 719 on 3 and 196 DF, p-value: < 2.2e-16
```

Recall that the above output says that the estimated model is:

$$sales = 1.288 + 0.07844TV - 0.0001136TV^2 + 0.193radio + error$$

Below we use the notation  $y = f(x) + \epsilon = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + \epsilon$ .

In our Advertising example, p = 3,  $x_1 = TV$ ,  $x_2 = TV^2$  and  $x_3 = radio$ . The sample size n = 200.

### Residuals

Recall that the residual is the estimated error.

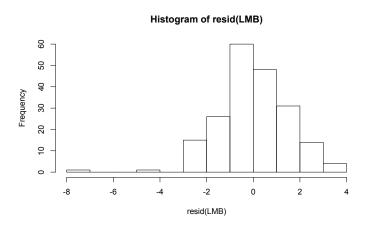
When the model is  $y = f(x) + \epsilon$  and  $\hat{f}$  is the estimated f, the estimated error  $\hat{\epsilon}$  is defined by  $y = \hat{f}(x) + \hat{\epsilon}$ .

```
Residuals:
Min 1Q Median 3Q Max
-7.3860 -0.8822 -0.0498 0.9613 3.5725
hist(resid(LMB))
```

The R otuput includes some statistics on the distribution of the residuals.

- The minimum of the residuals is -7.3860.
- The 1st quartile of the residuals is -0.8822.
- The median of the residuals is -0.0498.
- The 3rd quartile of the residuals is 09613.
- The maximum of the residuals is 3.5725.

Figure: The histogram of the resudials.



### Residual standard error

A linear regression estimated by least square assumes that  $\epsilon$  follows a distribution with mean 0 and a standard deviation  $\sigma$ .

Residual standard error: 1.517 on 196 degrees of freedom

R output indicates that estimated standard deviation  $\hat{\sigma}$  is 1.517. This is calculated by

$$\hat{\sigma}^2 = \frac{1}{n - p - 1} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_1 \cdots - \beta_p x_p)^2$$
 (1)

When we assume that  $\epsilon$  follows  $N(0, \sigma^2)$ ,  $\hat{\epsilon}/\hat{\sigma}$  follows a t-distribution with 196 degrees of freedom.

7/66

Shinki (Wayne State U) STA 5820 Chapter 3

#### Remark:

 $\epsilon$  and  $\hat{\epsilon}$  have different distributions.

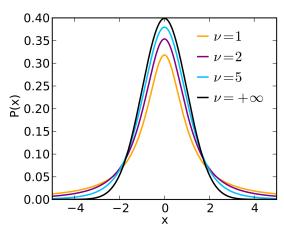
For example, imagine a linear regression

$$y = \beta_0 + \beta_1 x + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

with two observations  $(x_1, y_1), (x_2, y_2)$ .

Since we can always determine the line which goes through any two points, the residuals are always zero but errors are almost always non-zero.

The t-distribution is a symmetric distribution whose tails are fatter than a normal distribution. The figure shows the density of t-distribution for several different degrees of freedom. t-distribution with  $\infty$  degrees of freedom is a standard normal distribution.



### R<sup>2</sup>: Coefficient of determination

Multiple R-squared: 0.9167, Adjusted R-squared: 0.9154

The  $R^2$  is called coefficient of determinanation, and represents the ratio of sum of squared errors explained by predictors.

There are two versions. These are calculated as:

Multiple 
$$R^2 = 1 - \frac{SS_{Err}}{SS_{Tot}}$$
  
Adjusted  $R^2 = 1 - \frac{SS_{Err}/(n-p-1)}{SS_{Tot}/(n-1)}$ 

where **p** is the number of predictors (except intercept) and

$$SS_{Err} := (Y - X\hat{\beta})'(Y - X\hat{\beta}) = \sum (y_i - x_i\hat{\beta})^2$$
  

$$SS_{Tot} := (Y - \bar{Y})'(Y - \bar{Y}) = \sum (y_i - \bar{y})^2,$$

where  $\bar{\mathbf{Y}}$  is an n by 1 vector whose components are all  $\bar{\mathbf{y}}$ .

In short, the multiple  $\mathbb{R}^2$  is just a ratio, while the adjusted  $\mathbb{R}^2$  penalizes a large number of predictors for a fair comparison of models with a different number of predictors.

To be concrete, the expectation of the adjusted  $R^2$  is always zero when all predictors do not have any true relationship with y.

 ${\it R}^2$  is always between 0 and 1, and tends to be larger when the number of predictors becomes large (even if there are no true relationship between  ${\it x}$  and  ${\it y}$ ).

### Coefficient of determination and correlation coefficient

When there is only one predictor x, the coefficient of determination  $R^2$  is equal to the square of correlation coefficient r between x and y.

### F-test

```
F-statistic: 719 on 3 and 196 DF, p-value: < 2.2e-16
```

This is the result for a hypothesis testing:

- A null hypothesis  $H_0$ :  $\beta_1 = \beta_2 = \cdots = \beta_p = 0$  (i.e., the regression model is not useful at all), against
- an alternative hypothesis  $H_1$ :  $\beta_j \neq 0$  for some j.

The test statistic **F** is given by

$$F = \frac{(SS_{Tot} - SS_{Err})/p}{SS_{Err}/(n-p-1)}.$$
 (2)

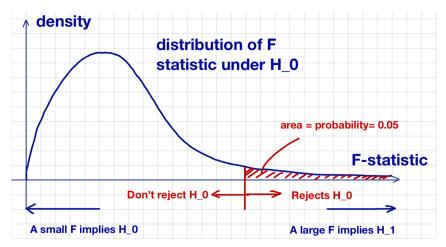
The value of F is larger when  $SS_{Err}$  gets smaller compared to  $SS_{Tot}$ .

Since  $SS_{Err}$  is the error size of regression model and  $SS_{Tot}$  is the total variability of y, this happens only if the regression model works good.

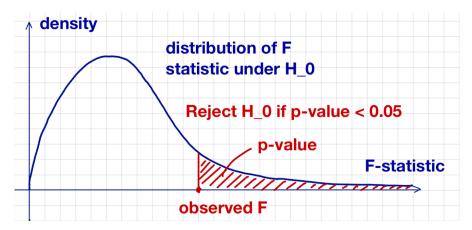
Therefore, we reject the null hypothesis when the value of **F** is larger than some threshold value.

Shinki (Wayne State U)

### An illustration of **F**-test:



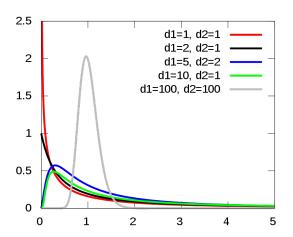
An illustration for **p**-value in **F**-test:



It is known that F follows an F-distribution with degrees of freedom (p, n - p - 1) under  $H_0$ .

An **F**-distribution has two parameters ("numerator degrees of freedom" and and "denominator degrees of freedom"), and its shape depends on the two parameters.

Figure: A graph of F-distributions.



F-statistic: 719 on 3 and 196 DF, p-value: < 2.2e-16

The R output indicates that F-statistic is 196, and it follows an F distribution with df = (3, 196) under  $H_0$ .

Since p-value =  $2 \cdot 10^{-16} < 0.05$ ,  $H_0$  is rejected.

The regression model is useful to explain y-value.

A linear model with least square estimation assumes

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \epsilon, \quad \epsilon \sim N(0, \sigma^2) \text{ IID}$$
 (3)

where IID means "independent and identically-distributed".

There are seveal possible violation of assumptions:

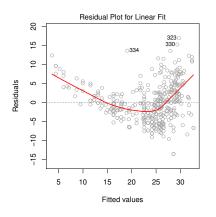
- Non-linearity of the response-predictor relationships.
- Correlation of error terms.
- Non-constant variance of error terms (heteroskedasticity).
- Outliers.
- High-leverage points.
- Collinearity.

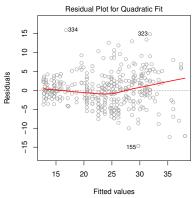
Shinki (Wavne State U) STA 5820

## **Non-linearity**

When residual plots have some (non-linear) patterns in trend, it implies that more information can be extracted from x to explain y. That is, there is non-linear relationship between x and y.

Figure 3-9: Left: residual plots of  $mpg = \beta_0 + \beta_1 HP + \epsilon$ . Right: residual plots of  $mpg = \beta_0 + \beta_1 HP + \beta_2 HP^2 + \epsilon$ .





### Remedies for non-linearity

- Transform  $\mathbf{x}$ ,  $\mathbf{y}$ , or both. Common functions used are  $\log(\mathbf{x})$ ,  $\mathbf{x}^{\alpha}$  with some  $\alpha$ .
- Add more predictors in the linear model. E.g.,  $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$ .

### Correlation of error terms

When  $\epsilon$  is correlated each other, standard errors of parameter estimates are underestimated.

Figure: Two series x and y are time series data with high auto-correlation (that is, adjacent observations such as  $x_t$  and  $x_{t+1}$  are highly correlated). Two series are similar by coincidence (actually two paths are independent random walks).

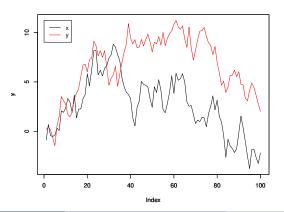
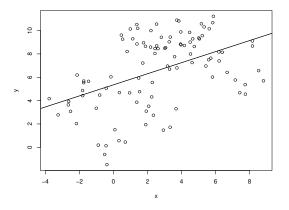


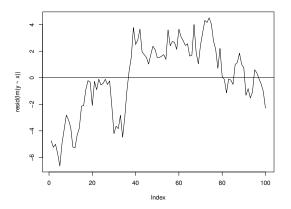
Figure: However,  $(x_t, y_t)$  looks highly related when we ignore time structure.



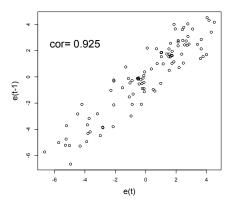
As a result, Im function returns a highly significant coefficient.

The problem: Independent assumption of  $\epsilon$  is clearly violated.

Figure: Residuals by time order



Correlation between  $\hat{\epsilon}_t$  and  $\hat{\epsilon}_{t-1}$  is 0.925, very high.



### Remedies for correlation of error terms

- Take the first difference  $\Delta x_t := x_t x_{t-1}$  of the time series (for both  $x_t$  and  $y_t$ ). It often removes time correlation.
- Estimate parameters with accounting for correlation between errors (generalized least square, GLS).

GLS gives more reasonable standard errors for parameters:

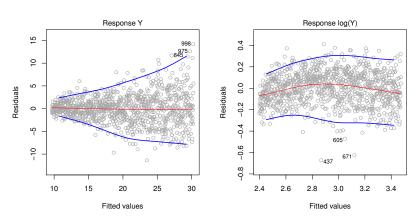
```
> library(nlme) # for qls
> GLS1 <- qls(v~x, correlation=corAR1())</pre>
> summary(GLS1)
Generalized least squares fit by REML
  Data: NULL
      AIC BIC logLik
  285.2752 295.615 -138.6376
Parameter estimate(s):
     Phi
0.9808276
Coefficients:
               Value Std.Error t-value p-value
(Intercept) 3.752359 3.549629 1.057113 0.2931
x
            0.133462 0.084324 1.582719 0.1167
Correlation:
  (Intr)
x = 0.012
Residual standard error: 4.966842
Degrees of freedom: 100 total; 98 residual
```

### Non-constant variance of error terms

 $\epsilon_1, \cdots, \epsilon_n$  may have different variances.

Namely,  $\epsilon_i \sim N(0, \sigma_i^2)$  and  $\sigma_i$  depends on i.

Example 1: (Left:) Residual plot indicates error size is larger for larger fitted values. (Right:) After transforming **Y** by logarithm, residual plot has equal variance.



### Example 2:

Suppose that you want to investigate relationship between height and weight of college students, and collected mean height and mean weight data from each of 100 colleges. There are 100 data points, but errors are not expected identially distributed. A small error in height-weight relationship is expected for colleges with a larger enrollment.

You may use a different estimation procedure such as weighted least square, WLS.

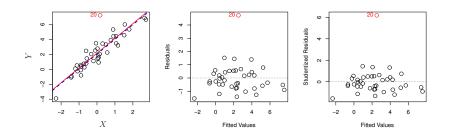
### Remedies for non-constant variance of error terms

- Transform the response variable  $\mathbf{y}$ . Common functions are  $\log \mathbf{y}$ ,  $\mathbf{y}^{\alpha}$  with some  $\alpha$ .
- Use an appropriate estimation method such as weighted least square.
- For time series data with different error size by time period, use models such as GARCH.

### **Outliers**

There are sometimes extremely large errors, called <u>outliers</u>. This violates normality assumtpion of errors. Also this makes estimates more unreliable.

Example: The 20th observations is an outlier.



Note: Standardized residual adjusts the size of errors by its expected size of errors. A residual tends to be larger when it is closer to the center in predictor value.

#### Remedies for outliers

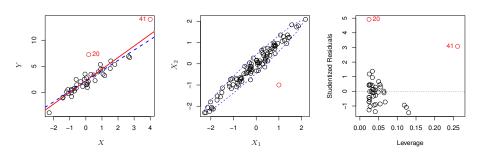
- Check if any recording errors in data collection.
- Check if the estimation is robust. Does the result change if the outlier(s) are dropped?
- Use a more robust estimation method (e.g., quantile regression, M-estimation).

#### **High Leverage points**

When the  $\mathbf{x}$  value of an observation is far away from the center, it may have too much influence on the regression line.

This is not good since a few observations almost determines the regression result. Often such observations may have larger errors than the other observations.

Figure: The 41st observation is influential point (left and right). An influential point may not be extreme in any specific predictor (center).



The leverage statistic of an observation  $(x_i, y_i)$  is given by

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{j=1}^n (x_j - \bar{x})^2}.$$

for a simple linear regression. (The formula for multiple regressions is different.)

 $h_i$  is between 1/n and 1, and the mean leverage is (p+1)/n where p is the number of predictors.

Shinki (Wayne State U)

#### Remedies for high leverage

- Transformation of x (or both x and y) may make the point less influential.
- Check if the estimation is robust. Does the result change if the outlier(s) are dropped?
- Separate influential points from the others, and use another model for them.

#### Collinearity

When some predictors  $x_1, \dots, x_q$  are nearly linearly dependent, we say there is collinearity in predictors.

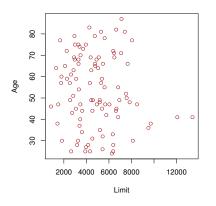
This fact inflates the standard errors of estimated coefficients, making more predictors look less significant.

Example: Credit Data

Want to regress 'balance' on

- 'age' and 'limit', where the two variable are almost independent.
- 'rating' and 'limit', where the two variable are highly dependent.

Figure: Credit Data



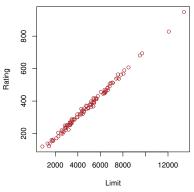
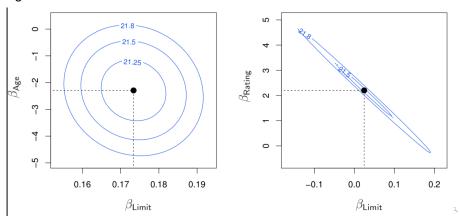


Table: Estimation results. Since 'rating' and 'limit' are highly correlated, it is hard to distinguish the effects from the two variables. Consequently, standard errors of the coefficients are larger in Model 2.

		Coefficient	Std. error	t-statistic	p-value
Model 1	Intercept	-173.411	43.828	-3.957	< 0.0001
	age	-2.292	0.672	-3.407	0.0007
	limit	0.173	0.005	34.496	< 0.0001
Model 2	Intercept	-377.537	45.254	-8.343	< 0.0001
	rating	2.202	0.952	2.312	0.0213
	limit	0.025	0.064	0.384	0.7012

**TABLE 3.11.** The results for two multiple regression models involving the Credit data set are shown. Model 1 is a regression of balance on age and limit, and Model 2 a regression of balance on rating and limit. The standard error of  $\hat{\beta}_{\text{limit}}$  increases 12-fold in the second regression, due to collinearity.

Figure: Confidence regions (2-dimensional version of confidence interval) of the two regression models above. (Left:) Model 1. Confidence interval for  $\beta_{Limit}$  is very narrow (consider project the contour on to x-axis). (Right:) Model 2. Confidence intervals for  $\beta_{Limit}$  is very wide, while the confidence region is still small in area.



The Variance Inflation Factor (VIF) represents how many times  $\mathrm{Var}\hat{\beta}_j$  gets larger (relative to squared residual standard error) when the model changes from  $\mathbf{y} = \beta_0 + \beta_j \mathbf{X}_j + \epsilon$  to  $\mathbf{y} = \beta_0 + \beta_1 \mathbf{X}_1 + \cdots + \beta_p \mathbf{X}_p + \epsilon$ .

$$VIF(\hat{\beta}_j) = \frac{1}{1 - R_{X_j|X_{-j}}^2}$$

where  $R_{X_j|X_{-j}}^2$  is the multiple  $R^2$  when  $X_j$  is regressed on the other predictors.

When VIF is more than 10, multicollinearity is regarded as severe.

Shinki (Wayne State U)

#### Example of VIF:

Regress balance on Limit and two other predictors, and evaluate the standard error of the coefficient of Limit.

```
> summary(lm(Balance ~ Limit))
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -2.928e+02 2.668e+01 -10.97 <2e-16 ***
Limit
       1.716e-01 5.066e-03 33.88 <2e-16 ***
Residual standard error: 233.6 on 398 degrees of freedom
> summary(lm(Balance ~ Age + Rating + Limit))
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -259.51752 55.88219 -4.644 4.66e-06 ***
       -2.34575    0.66861    -3.508    0.000503 ***
Age
Rating 2.31046 0.93953 2.459 0.014352 *
Limit
           0.01901 0.06296 0.302 0.762830
Residual standard error: 229.1 on 396 degrees of freedom
```

The standard error for Limit inflated from 0.005066 (simple regression) to 0.06296 (multiple regression). Relative to residual standard error, the ratio is

$$\frac{0.06296/229.1}{0.005066/233.6} = 12.67.$$

If we consider the ratio of variances,  $12.67^2 = 160.58$ . This is obtained by

The VIF can also be calculated directly by definition.

```
> R2 <- summary(lm(Limit ~ Age + Rating))$r.squared #$
> 1/(1-R2) # VIF
[1] 160.5929
```

#### Remedies for collinearity

- Ignore the issue if you only focus on prediction.
- Exclude similar predictors beforehand.
- Combine similar predictors beforehand (e.g., principal component analysis, state space models).
- Use a variable selection method which drops more variables (e.g., Lasso, ridge regression).

#### **Example: Property Sales and the number of bedrooms**

Consider a forecasting problem for sales in the Property Sales Data in Troy, MI. Sales may depend on the number of bedrooms. The number of bedrooms is either 0,2,3,4,5 or 6, so it can be regarded as either quantitative or qualitative variables.

Consider the following models:

Price = 
$$\beta_0 + \beta_1 \operatorname{Sqft} + \beta_2 \operatorname{Year} + \beta_3 \operatorname{Bath} + \beta_4 \operatorname{Bed} + \epsilon$$
 (4)

Price = 
$$\beta_0 + \beta_1 \operatorname{Sqft} + \beta_2 \operatorname{Year} + \beta_3 \operatorname{Bath} + \beta_4 \operatorname{Bed} + \beta_{4,i} + \epsilon_{ij}$$
 (5)

#### where

- Bed is a quantitative variable, and
- $\beta_{4,i}$  represents a factor (dummy variable) for i bedrooms (i = 2, 3, 4, 5, 6) as 0 bedroom as a baseline. (Note: One of the 5 factors is redundant because there are 6 parameters ( $\beta_4, \beta_{4,2}, \dots, \beta_{4,6}$ ) to represent 5 levels other than the baseline.)
- The first model assumes that the price change for one additional bedroom is constant, while the second model assumes a non-linear relationship between price and the number of bedrooms.

Shinki (Wayne State U) STA 5820 Chapter 3 54/66

#### Sample R code:

```
> LM.1 <- lm(Price ~ Sqft+Year+Bath+Bed) # model (3)</pre>
```

- > Bed.f <- as.factor(Bed) # Number of Bedroom as factor</pre>
- > LM.f <- lm(Price ~ Sqft+Year+Bath+Bed+Bed.f) # model (4)</pre>

#### Results for the model (4):

The number of bedrooms is a significant factor (p-value = 0.00548).

#### Results for the model (5):

```
> summary(LM.f)
Coefficients: (1 not defined because of singularities)
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -1699196.6 251265.9 -6.763 3.94e-11 ***
                           4.2 26.613 < 2e-16 ***
Sqft
               111.8
               833.7 126.7 6.581 1.22e-10 ***
Year
              9902.4
                        3907.2 2.534 0.01158 *
Bath
Bed
            -31086.1 7275.5 -4.273 2.33e-05 ***
Bed.f2
            83608.0 23314.3 3.586 0.00037 ***
Red. f3
            109130.7 22260.2 4.903 1.30e-06 ***
            125143.1 27276.6 4.588 5.72e-06 ***
Bed.f4
            168758.0 37235.0 4.532 7.37e-06 ***
Bed. f5
Bed. f6
                  NΑ
                            NA
                                   NΑ
                                           NΑ
Residual standard error: 39730 on 481 degrees of freedom
Multiple R-squared: 0.835, Adjusted R-squared: 0.8322
F-statistic: 304.2 on 8 and 481 DF, p-value: < 2.2e-16
```

The above result indicates:

when we introduce a paremeter for each level of **Bed**, many of them are significant predictors of **Price**.

The following ANOVA table can test the overall significance of the factor:

```
Analysis of Variance Table

Response: Price

Df Sum Sq Mean Sq F value Pr(>F)

Sqft 1 3.7140e+12 3.7140e+12 2352.7231 < 2.2e-16 ***

Year 1 6.0205e+10 6.0205e+10 38.1382 1.404e-09 ***

Bath 1 1.2500e+10 1.2500e+10 7.9184 0.005094 **

Bed 1 1.2853e+10 1.2853e+10 8.1424 0.004511 **

Bed.f 4 4.1659e+10 1.0415e+10 6.5976 3.562e-05 ***

Residuals 481 7.5930e+11 1.5786e+09

---

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The table reads: after accounting for **Sqft**, **Year**, **Bath** and **Bed** as continuous variables, **Bed.f** is a sigfinicant factor in the model (p-value =  $3.562 \times 10^{-5}$ ).

> anova(LM.f)

AIC also indicates the model (5) is a better prediction model.

```
> AIC(LM.1) # model (3)
[1] 11797.75

> AIC(LM.f) # model (4)
[1] 11779.58
```

#### Note:

The same analysis can be done for the number of bathrooms. In fact, the number of bathrooms as a factor is also a significant predictor of price. (The result is not shown in slides.)

## 3.d Removing additive assumption

#### Removing additive assumption

Suppose we want to predict Y by  $X_1$  and  $X_2$ . A basic multiple linear regression is:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

This model assumes that  $X_1$  and  $X_2$  do not have interaction. A model with an interaction term is:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \epsilon$$

Shinki (Wayne State U)

## 3.d Removing additive assumption

#### **Example 1: Sales and advertising**

	Coefficient	Std. error	t-statistic	p-value
Intercept	6.7502	0.248	27.23	< 0.0001
TV	0.0191	0.002	12.70	< 0.0001
radio	0.0289	0.009	3.24	0.0014
TV×radio	0.0011	0.000	20.73	< 0.0001

TABLE 3.9. For the Advertising data, least squares coefficient estimates associated with the regression of sales onto TV and radio, with an interaction term, as in (3.33).

## 3.d Removing additive assumption

#### Other examples:

- Crop yield may be affected by the amount of fertilizer only when sunlight is not enough.
- Southpaws pitch well only when the batter is left-handed.

## 3.e KNN and linear regression

Remember K-Nearest neighborhood (KNN) method, which use K closest observations to determine the predicted value at x.

While it is used for categorization problem in Chapter 2, it can also be used for regression problem. To be exact, define the fitted value at  $x_0$  by

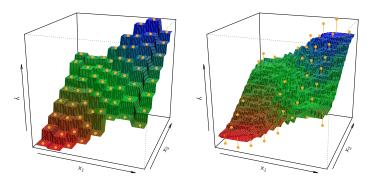
$$\hat{f}(x_0) = \frac{1}{K} \sum_{x_0 \in N_0} y_i$$

where  $N_0$  is a set of the K closest points to  $x_0$  within the data set.

Shinki (Wayne State U)

# 3.e KNN and linear regression

Figure illustrates KNN in regression problems with two predictors  $x_1$  and  $x_2$  (left: K = 1; right: K = 9).



KNN is more flexible in the shape of  $\hat{\textbf{f}}$  than linear regression, while it lacks features such as significant of regression coefficients.

#### Memo