# STA302/1001: Methods of Data Analysis

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Chapter 3: Multiple Linear Regression

# Multiple Linear Regression

- generalizes the simple linear regression model by allowing more terms than just the intercept and slope
- a simple example

$$\mathrm{E}(Y|X_1 = x_1, X_2 = x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$
$$\mathrm{Var}(Y|X_1 = x_1, X_2 = x_2) = \sigma^2$$

- main question: will the adding of $X_2$ help $\mathrm{E}(Y|X_1 = x_1)$?
- if yes, how much?

# Multiple Linear Regression - Con't

- Unite Nations data in Section 3.1 of text
  - Fertility: birth rate per 1000 females in 2000
  - PPgdp: per person gross domestic product in 2001
  - Purban: percentage of urban population
  - Locality: 193 regions
- $Y$: log(Fertility) $X_1$: log(PPgdp), $X_2$: Purban

$$R^2 = 46\% \quad \text{for} \quad \widehat{\mathrm{E}(Y|X_1)} = 2.703 - 0.153x_1$$

$$R^2 = 35\% \quad \text{for} \quad \widehat{\mathrm{E}(Y|X_2)} = 1.750 - 0.013x_2$$

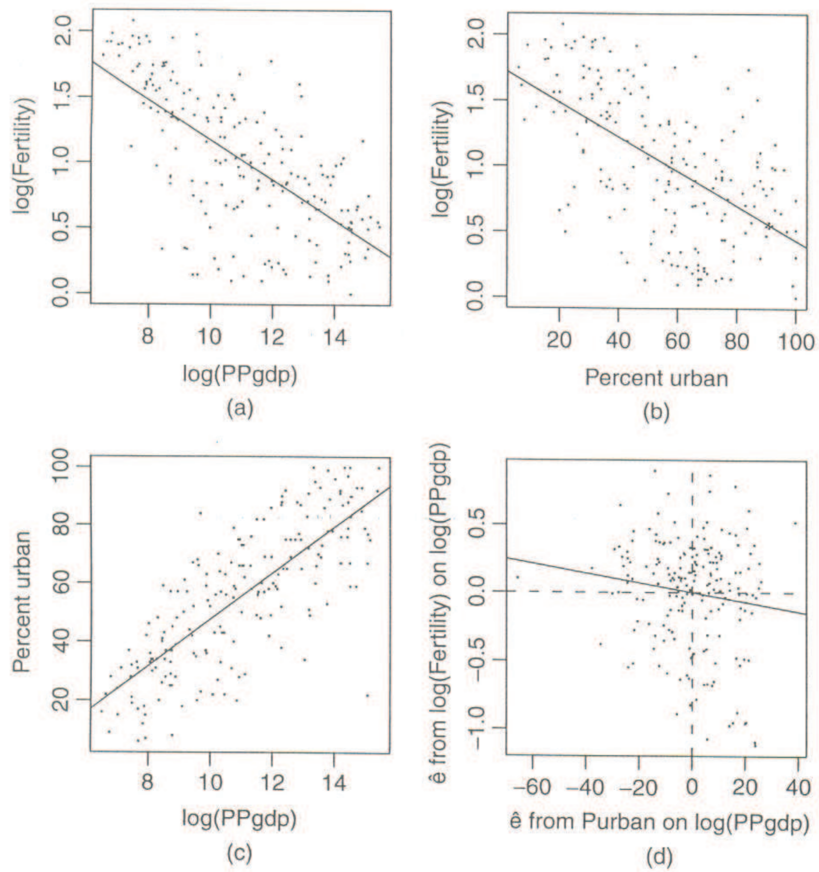
- higher PPgdp or Purban leads to lower birth rate
- what if we consider both $X_1$ and $X_2$ in regression?

# Multiple Linear Regression - Con't

- for $E(Y|X_1, X_2)$: $R^2 = 46\% + 35\%$ only if $X_1$ and $X_2$ are completely unrelated and measure different things.
  Q: will this be the case for UN data?
- more often situation: $46\% \leq R^2 \leq 46\% + 35\%$
- how much additional explanation was offered by $X_2$?
- let $\hat{e}_{Y|X_1}$ be the residuals of regressing $Y$ on $X_1$:
  variability of $Y$ not explained by $X_1$, or variability of $Y$ after the effect of $X_1$ is removed
- let $\hat{e}_{X_2|X_1}$ be the residuals of regressing $X_2$ on $X_1$:
  variability of $X_2$ not explained by $X_1$, or variability of $X_2$ after the effect of $X_1$ is removed

# Added-Variable Plot

- regression and residual plots: (b) v.s. (d)
  $\hat{\beta}_2 = -0.013$ ignoring $X_1$, $\hat{\beta}_2 = -0.004$ adjusting for $X_1$



# Multiple Linear Regression (MLR)

- in general, multiple linear model:

$$\mathrm{E}(Y|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

$$\mathrm{Var}(Y|X) = \sigma^2$$

- a linear function of the parameters $\{\beta_0, \ldots, \beta_p\}$
- $p = 1 \Rightarrow$ simple linear regression
- when $p = 2$, fit a 2D plane in a 3D space

# Regression Surface for $p = 2$

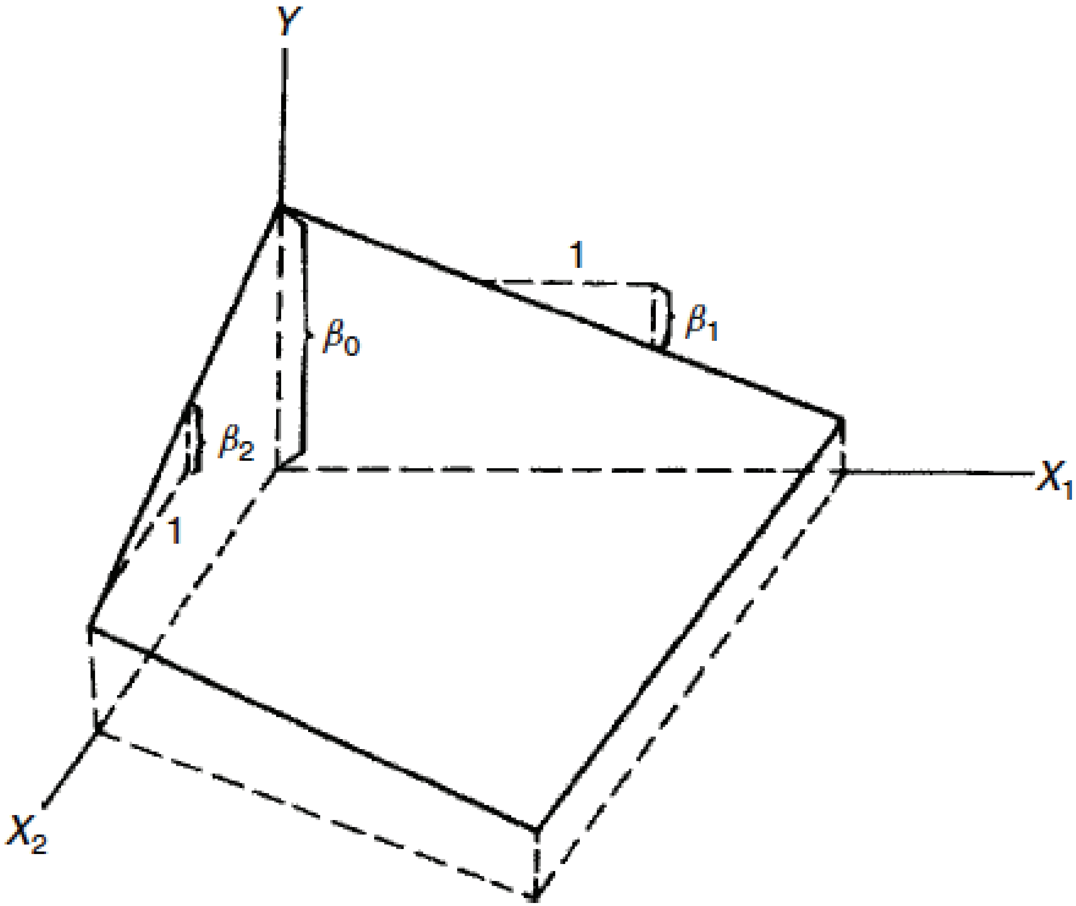



**FIG. 3.2** A linear regression surface with $p = 2$ predictors.

# Terms and Predictors

- the textbook distinguishes “predictors” and “terms”, only for convenience and to avoid confusion
- predictors: the "original data that you collect"
- e.g., height, weight, color, smoking or not
- terms: created from predictors, the $X$-variable in our multiple regression models
- e.g., height$^2$, $\log($weight$)$, height $\times$ weight, color, ...
- an important question in multiple linear regression:
  *the selection of a "good" set of terms*

# Matrix Notation for MLR

- Recall: $\mathrm{E}(Y|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$
  $\mathrm{Var}(Y|X) = \sigma^2$
- observed values:
$$\begin{array}{c}(x_{11}, x_{12}, \cdots, x_{1p}, y_1)\\ (x_{21}, x_{22}, \cdots, x_{2p}, y_2)\\ \vdots \qquad\qquad \vdots\\ (x_{n1}, x_{n2}, \cdots, x_{np}, y_n)\end{array}$$
- $$\mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \qquad \mathbf{X} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1p} \\ 1 & x_{21} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{pmatrix}$$

# Matrix Notation for MLR - Con't

- the $i$th row of $\mathbf{X}$ will be denoted as $\mathbf{x}_i'$
- $$\boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} \qquad \mathbf{x}_i = \begin{pmatrix} 1 \\ x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix} \qquad \mathbf{e} = \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{pmatrix}$$
- there are $(p+1)$ parameters, including the intercept $\beta_0$

# Matrix Notation for MLR - Con't

- multiple linear regression in matrix notation

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

- the $i$th row is $y_i = \mathbf{x}_i'\boldsymbol{\beta} + e_i$

  $\Rightarrow y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + e_i$

- about the vector of errors $\mathbf{e}$:

$$\mathrm{E}(\mathbf{e}) = \mathbf{0}, \qquad \mathrm{Var}(\mathbf{e}) = \sigma^2 \mathbf{I_n}$$

- if we add normality assumption:

$$\mathbf{e} \sim \mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I_n})$$

# OLS for Multiple Linear Regression

- $RSS(\boldsymbol{\beta}) = \sum_{i=1}^{n}(y_i - \mathbf{x}_i'\boldsymbol{\beta})^2 = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$
- if $(\mathbf{X}'\mathbf{X})^{-1}$ exists, $RSS(\boldsymbol{\beta})$ is minimized by

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

- $\mathbf{X}'\mathbf{X}$, $\mathbf{X}'\mathbf{Y}$: similar to $SXX$, $SXY$
- Residuals: $\hat{\mathrm{e}} = \mathbf{Y} - \hat{\mathbf{Y}}$
- $RSS = \hat{\mathbf{e}}'\hat{\mathbf{e}} = (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})'(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})$
- $\sigma^2 = \mathrm{Var}(Y|X)$ is estimated with $\hat{\sigma}^2 = \frac{RSS}{n-(p+1)}$
- with the normality assumption we have

$$(n - (p+1))\hat{\sigma}^2/\sigma^2 \sim \chi^2(n - (p+1))$$

# OLS using Matrices

- model: $\mathrm{E}(Y|X=\mathbf{x}) = \boldsymbol{\beta}'\mathbf{x}$ and $\mathrm{Var}(Y|X=\mathbf{x}) = \sigma^2$
- OLS estimates $\hat{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}$ minimize
  $RSS(\boldsymbol{\beta}) = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$
  $= \mathbf{Y}'\mathbf{Y} + \boldsymbol{\beta}'(\mathbf{X}'\mathbf{X})\boldsymbol{\beta} - 2\mathbf{Y}'\mathbf{X}\boldsymbol{\beta}$
- some matrix differentiation results to proceed:

$$\frac{\partial \boldsymbol{c}\boldsymbol{\beta}}{\partial \boldsymbol{\beta}} = \boldsymbol{c}' \quad \text{and} \quad \frac{\partial \boldsymbol{\beta}'\boldsymbol{V}\boldsymbol{\beta}}{\partial \boldsymbol{\beta}} = (\boldsymbol{V} + \boldsymbol{V}')\boldsymbol{\beta}$$

- by setting the derivative of $RSS(\boldsymbol{\beta})$ to zero, we have
  normal equation: $\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{Y}$
- thus the OLS estimate is $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$

# Properties of OLS Estimates

- assume $\mathrm{E}(\mathbf{e}) = \mathbf{0}$ and $\mathrm{Var}(\mathbf{e}) = \sigma^2 \mathbf{I}_n$, $\hat{\beta}$ is unbiased

$$\mathrm{E}(\hat{\boldsymbol{\beta}}|\mathbf{X}) = \mathrm{E}((\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}|\mathbf{X})$$
$$= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathrm{E}(\mathbf{Y}|\mathbf{X})$$
$$= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta}$$
$$= \boldsymbol{\beta}$$

- for variance, we will need $\mathrm{Var}(\boldsymbol{B}'\boldsymbol{Z}) = \boldsymbol{B}'\mathrm{Var}(\boldsymbol{Z})\boldsymbol{B}$

$$\mathrm{Var}(\hat{\boldsymbol{\beta}}|\mathbf{X}) = \mathrm{Var}((\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}|\mathbf{X})$$
$$= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'[\mathrm{Var}(\mathbf{Y}|\mathbf{X})]\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$$
$$= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'[\sigma^2\mathbf{I}_n]\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$$
$$= \sigma^2(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$$
$$= \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$$

# Residual Sum of Squares

- $$\begin{aligned} RSS = RSS(\hat{\boldsymbol{\beta}}) &= (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})'(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &= \mathbf{Y}'\mathbf{Y} + \hat{\boldsymbol{\beta}}'(\mathbf{X}'\mathbf{X})\hat{\boldsymbol{\beta}} - 2\mathbf{Y}'\mathbf{X}\hat{\boldsymbol{\beta}} \end{aligned}$$
- $\hat{\boldsymbol{\beta}}'(\mathbf{X}'\mathbf{X})\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}'(\mathbf{X}'\mathbf{X})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{Y} = \mathbf{Y}'\mathbf{X}\hat{\boldsymbol{\beta}}$
- $RSS = \mathbf{Y}'\mathbf{Y} - \hat{\boldsymbol{\beta}}\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{Y}'\mathbf{Y} - \hat{\mathbf{Y}}'\hat{\mathbf{Y}}$, with $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$
- why does this satisfy the pythagorean property?
- $$\begin{aligned} \mathbf{X}'\hat{\mathbf{e}} = \mathbf{X}'(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) &= \mathbf{X}'\mathbf{Y} - \mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} \\ &= \mathbf{X}'\mathbf{Y} - \mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{0} \end{aligned}$$
- $\hat{\mathrm{e}}$ is orthogonal to column space of $\mathbf{X}$, denoted by $S(\mathbf{X})$
- $\hat{\mathbf{Y}} = \mathbf{X}\hat{\beta}$ is the projection of $\mathbf{Y}$ onto $S(\mathbf{X}) \Longrightarrow \hat{\mathbf{e}} \perp \hat{\mathbf{Y}}$

# Geometric Interpretation of OLS

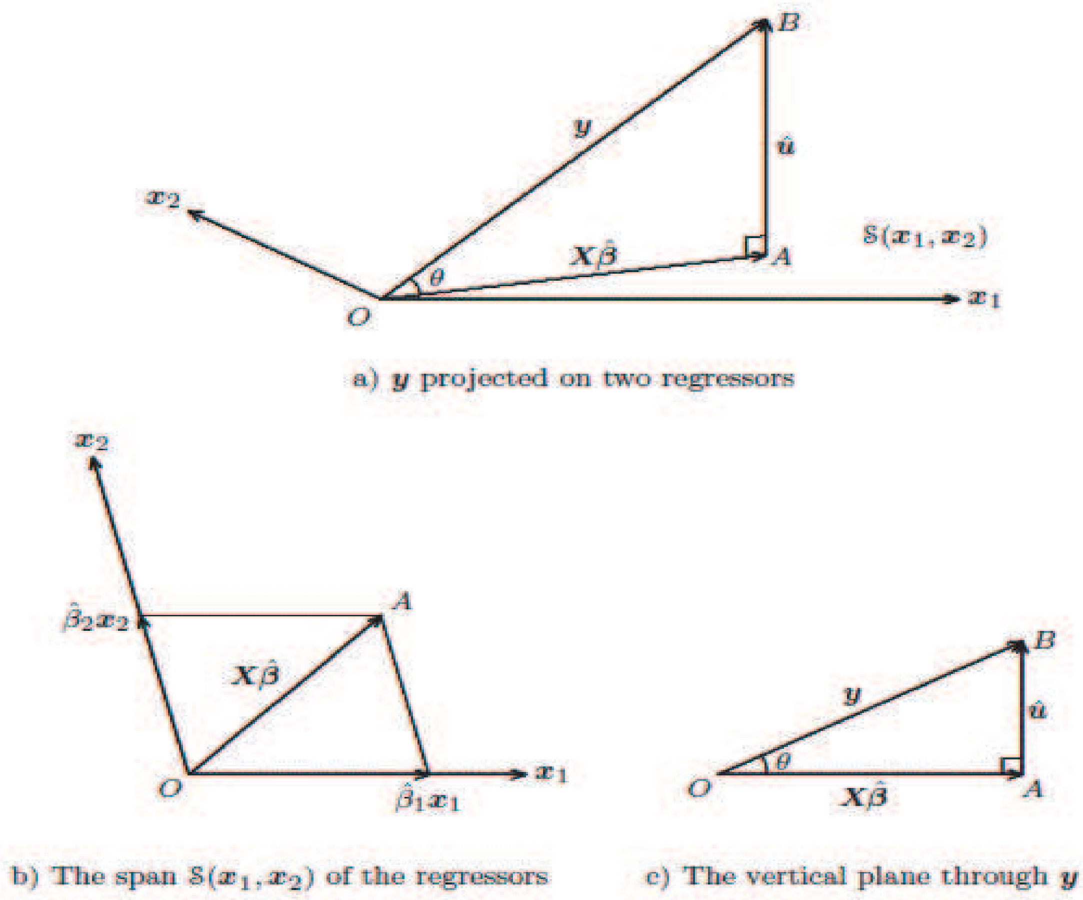


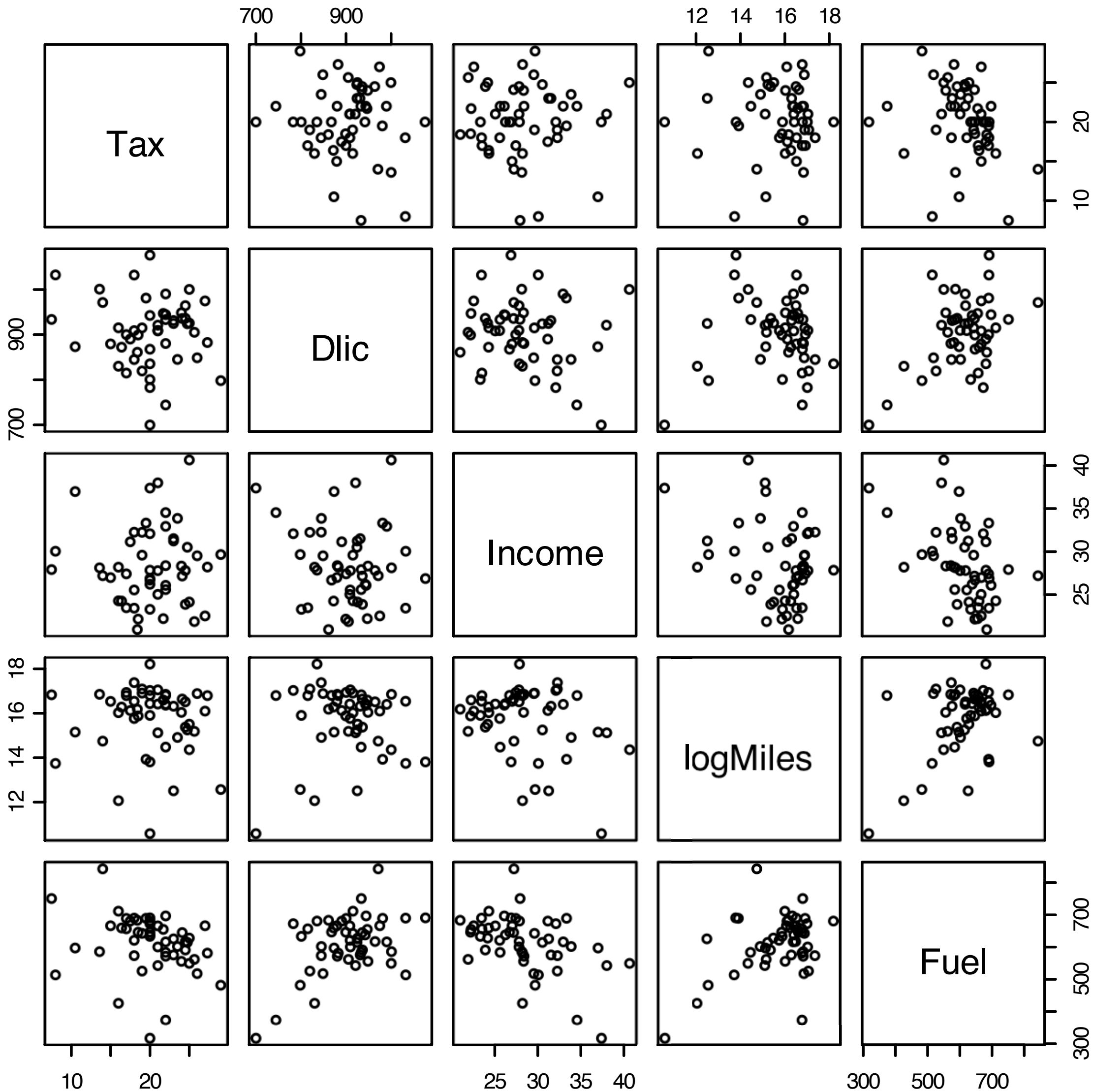

**Figure 2.11** Linear regression in three dimensions

- express the simple linear regression in matrix form

# Fuel Consumption Data

- goal: effect of gasoline tax on fuel consumption over U.S. states, including Washington D.C. (how many?)
- $Y$: Fuel, fuel consumption averaged over state population
- 4 terms:
  1. Tax: tax on gasoline in each state
  2. Dlic: number of driver licenses averaged over state population
  3. Income: personal income in each state
  4. logMiles: total length of highway in each state, in log miles (base two)

# Fuel Consumption Data - Con’t



# Fuel Consumption Data - Con't

TABLE 3.2 Sample Correlations for the Fuel Data

Sample Correlations

| | Tax | Dlic | Income | logMiles | Fuel |
|---|---|---|---|---|---|
| Tax | 1.0000 | -0.0858 | -0.0107 | -0.0437 | -0.2594 |
| Dlic | -0.0858 | 1.0000 | -0.1760 | 0.0306 | 0.4685 |
| Income | -0.0107 | -0.1760 | 1.0000 | -0.2959 | -0.4644 |
| logMiles | -0.0437 | 0.0306 | -0.2959 | 1.0000 | 0.4220 |
| Fuel | -0.2594 | 0.4685 | -0.4644 | 0.4220 | 1.0000 |

# Fuel Consumption Data - Con't

- the linear regression model to be fitted
  $\mathrm{E}(\mathrm{Fuel}|X) = \beta_0 + \beta_1 \mathrm{Tax} + \beta_2 \mathrm{Dlic} + \beta_3 \mathrm{Income} + \beta_4 \log(\mathrm{Miles})$

TABLE 3.3 Multiple Linear Regression for the Fuel Data

Coefficients

| | Estimate | Std. Error | t value | Pr(>\|t\|) |
|---|---|---|---|---|
| (Intercept) | 154.1928 | 194.9062 | 0.791 | 0.432938 |
| Tax | -4.2280 | 2.0301 | -2.083 | 0.042873 |
| Dlic | 0.4719 | 0.1285 | 3.672 | 0.000626 |
| Income | -6.1353 | 2.1936 | -2.797 | 0.007508 |
| logMiles | 18.5453 | 6.4722 | 2.865 | 0.006259 |

Residual standard error: 64.89 on 46 degrees of freedom
Multiple R-Squared: 0.5105
F-statistic: 11.99 on 4 and 46 DF, p-value: 9.33e-07

# ANOVA for Multiple Linear Regression

- Comparing
  $\mathrm{E}(Y|X=\mathbf{x}) = \beta_0 + \sum_{j=1}^{p} \beta_j x_j$ with $\mathrm{E}(Y|X=\mathbf{x}) = \beta_0$
- similar to simple linear regression

| The Analysis of Variance Table | | | | | |
|---|---|---|---|---|---|
| Source | df | SS | MS | F | p-value |
| Regression | $p$ | $SS_{reg}$ | $SS_{reg}/p$ | $MS_{reg}/\hat{\sigma}^2$ | |
| Residual | $n-(p+1)$ | $RSS$ | $\hat{\sigma}^2 = \frac{RSS}{n-(p+1)}$ | | |
| Total | $n-1$ | $SYY$ | | | |

# ANOVA for Fuel Consumption

- The test is:
  NH: $\mathrm{E}(Y|X=\mathbf{x}) = \beta_0$ vs AH: $\mathrm{E}(Y|X=\mathbf{x}) = \boldsymbol{\beta}'\mathbf{x}$

Fuel Consumption Data

| | Df | Sum Sq | Mean Sq | F value | Pr(>F) |
|---|---|---|---|---|---|
| Regression | 4 | 201994 | 50499 | 11.992 | 9.33e-07 |
| Residuals | 46 | 193700 | 4211 | | |
| Total | 50 | 395694 | | | |

- Coefficient of Determination
  $R^2 = \frac{SS_{reg}}{SYY} = \frac{SYY-RSS}{SYY} = 1 - \frac{RSS}{SYY}$
- $R^2 = \frac{201994}{395694} = 0.5105$ for fuel consumption

# Hypothesis Test for One Term

- Fuel Consumption: what will happen if we delete Tax from the model?
- NH: $\beta_1 = 0$, $\beta_0, \beta_2, \beta_3, \beta_4$ arbitrary
  AH: $\beta_1 \neq 0$, $\beta_0, \beta_2, \beta_3, \beta_4$ arbitrary
- fit a model with all terms: Model B (Bigger)
- fit a model with all terms but tax - Model S (smaller)
- Let $RSS_B$ be the $RSS$ from Model B
- let $RSS_S$ be the $RSS$ from Model S
- which is bigger? $RSS_S \geq RSS_B$ (why?)

# Hypothesis Test for One Term -con't

- $RSS_S$ - $RSS_B$ gives the "contribution" of Tax after adjusting all other terms

| | df | SS | MS | F | Pr(>F) |
|---|---|---|---|---|---|
| $RSS_S$ | 47 | 211964 | | | |
| $RSS_B$ | 46 | 193700 | 4211 | | |
| Difference | 1 | 18264 | 18264 | 4.34 | 0.043 |
| | | | (SS/df) | (MS/$\hat{\sigma}^2$) | |

- so for this problem, Tax is statistically significant
- this $F$-test for one term is the same as $t$-test ($t^2 = F$)

# Sequential Analysis of Variance Tables

- in Model B with Tax, Dlic, Income, logMiles, $SS_{reg} = 201994$ tells how much variation is explained
- for the smaller model (without Tax), $SS_{reg} = 201994$ from Model B is decomposed into two parts:
  1: "Dlic, Income, logMiles", $SS_{others} = 183730$
  2: "Tax, given Dlic, Income, logMiles" $SS_{tax} = 18264$
- we could continue this decomposition

  e.g., 1: "logMiles"
  2: "Income, given logMiles"
  3: "Dlic, given Income, logMiles"
  4: "Tax, given Dlic, Income, logMiles"

# Sequential Analysis of Variance Tables - Con't

- for the fuel example, 4 parts
- in general, the order of decomposition matters

(a) First analysis

| | Df | Sum Sq | Mean Sq |
|---|---|---|---|
| Dlic | 1 | 86854 | 86854 |
| Tax | 1 | 19159 | 19159 |
| Income | 1 | 61408 | 61408 |
| logMiles | 1 | 34573 | 34573 |
| Model B | 4 | 201994 | 50499 |
| Residuals | 46 | 193700 | 4211 |

(b) Second analysis

| | Df | Sum Sq | Mean Sq |
|---|---|---|---|
| logMiles | 1 | 70478 | 70478 |
| Income | 1 | 49996 | 49996 |
| Dlic | 1 | 63256 | 63256 |
| Tax | 1 | 18264 | 18264 |
| Model B | 4 | 201994 | 50499 |
| Residuals | 46 | 193700 | 4211 |

(terms entering the model from top to bottom)

# Predictions and Fitted Values

- similar to simple linear regression
- prediction: given a new $\mathbf{x}_*$, predict $\mathbf{y}_*$ with
- $\hat{\mathbf{y}}_* = \mathbf{x}_*{}'\hat{\boldsymbol{\beta}}$
- $\mathrm{sepred}(\hat{\mathbf{y}}_* - \mathbf{y}_* | \mathbf{x}_*) = \hat{\sigma}\sqrt{1 + \mathbf{x}_*{}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_*}$
- fitted value: given a value $\mathbf{x}$, want to estimate the mean function at $\mathbf{x}$
- $\hat{\mathrm{E}}(Y|X = \mathbf{x}) = \hat{\mathbf{y}} = \mathbf{x}'\hat{\boldsymbol{\beta}}$
- $\mathrm{sefit}(\hat{\mathbf{y}}|\mathbf{x}) = \hat{\sigma}\sqrt{\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}}$
- $\mathrm{sepred}(\hat{\mathbf{y}}_* - \mathbf{y}_* | \mathbf{x}) = \sqrt{\hat{\sigma}^2 + \mathrm{sefit}(\hat{\mathbf{y}}_*|\mathbf{x})^2}$