Scientific Computing for Biologists

Linear Algebra Review II & Multiple Regression

Instructor: Paul M. Magwene

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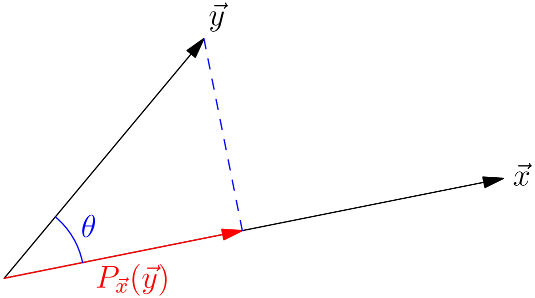
Overview of Lecture

- More Linear Algebra
  - Linear combinations and Spanning Spaces
  - Subspaces
  - Basis vectors
  - Dimension
  - Rank
- More on Regression
  - Multiple regression
  - Curvilinear regression
  - Major axis regression

Hands-on Session

- Literate Programming with R and knitr
- Multiple regression

A bit of review



$$\cos\theta = ?$$

$$P_{\vec{x}}(\vec{y}) = ? \qquad C_{\vec{x}}(\vec{y}) = ?$$

Space Spanned by a List of Vectors

Definition

Let X be a finite list of n-vectors. The **space spanned** by X is the set of all vectors that can be written as linear combinations of the vectors in X.

A space spanned includes the zero vector and is closed under addition and multiplication by a scalar.

Remember that a *linear combination* of vectors is an equation of the form $z = b_1 \mathsf{x}_1 + b_2 \mathsf{x}_2 + \cdots + b_p \mathsf{x}_p$

Subspaces

$\mathbb{R}^n$ denotes the seat of real n-vectors - the set of all $n \times 1$ matrices with entries from the set $\mathbb{R}$ of real numbers.

Definition

A **subspace** of $\mathbb{R}^n$ is a subset S of $\mathbb{R}^n$ with the following properties:

1. $0 \in S$
2. If $\mathsf{u} \in S$ then $k\mathsf{u} \in S$ for all real numbers k
3. If $\mathsf{u} \in S$ and $\mathsf{v} \in S$ then $\mathsf{u} + \mathsf{v} \in S$

Examples of subspaces of $\mathbb{R}^n$:

- any space spanned by a list of vectors in $\mathbb{R}^n$
- the set of all solution to an equation $A\mathsf{x} = 0$ where A is a $p \times n$ matrix, for any number p.

Basis

Let S be a subspace of $\mathbb{R}^n$. Then there is a finite list, X of vectors from S such that S is the space spanned by X.

Let S be a subspace of $\mathbb{R}^n$ spanned by the list $(u_1, u_2, \ldots, u_n)$. Then there is a linearly independent sublist of $(u_1, u_2, \ldots, u_n)$ that also spans S.

Definition

A list X is a **basis** for S if:

- X is linearly independent
- S is the subspace spanned by X

Dimension

Let S be a subspace of $\mathbb{R}^n$.

Definition

The **dimension** of S is the number of elements in a basis for S.

Rank of a Matrix

Let A by an $n \times p$ matrix.

Definition

The **rank** of A is equal to the dimension of the row space of A which is equal to the dimension of the column space of A.

Where the row space of A is the space spanned by the list of rows of A and the column space of A is defined similarly.

Equivalence Theorem

Let A by an $p \times p$ matrix. The following are equivalent

- A is singular
- the rank of A is less than p
- the columns of A form a LD list in $\mathbb{R}^n$.
- the rows of A form a LD list in $\mathbb{R}^n$
- the equation $A\mathsf{x} = 0$ has non-trivial solutions
- the determinant of A is zero

Regression Models

Variable space view of multiple regression

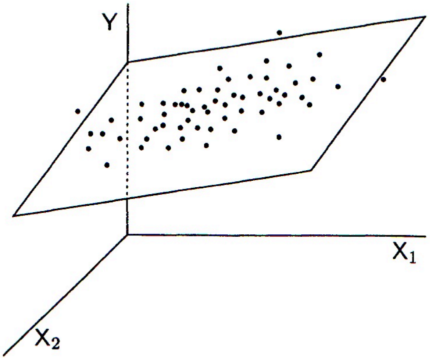
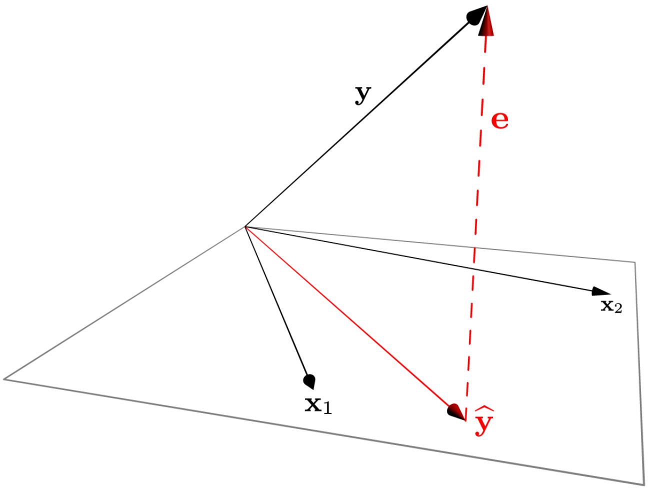


Figure 4.1: *The regression of* Y *onto* X_1 *and* X_2 *as a scatterplot in variable space.*

Subject Space Geometry of Multiple Regression



Multiple Regression

Let Y be a vector of values for the outcome variable. Let X_i be explanatory variables and let x_i be the mean-centered explanatory variables.

$$\mathsf{Y} = \hat{\mathsf{Y}} + e$$

where –

Uncentered version:

$$\hat{Y} = a\mathbf{1} + b_1\mathsf{X}_1 + b_2\mathsf{X}_2 + \cdots + b_p\mathsf{X}_p$$

Centered version:

$$\hat{y} = b_1\mathsf{x}_1 + b_2\mathsf{x}_2 + \cdots + b_p\mathsf{x}_p$$

Statistical Model for Multiple Regression

In matrix form:

$$\mathsf{y} = \mathsf{X}\mathsf{b} + \mathsf{e}$$

$$\mathsf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \ \mathsf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix};$$

$$\mathsf{b} = \begin{bmatrix} a \\ b_1 \\ b_2 \\ \vdots \\ b_p \end{bmatrix}; \ \mathsf{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

Estimating the Coefficients for Multiple Regression

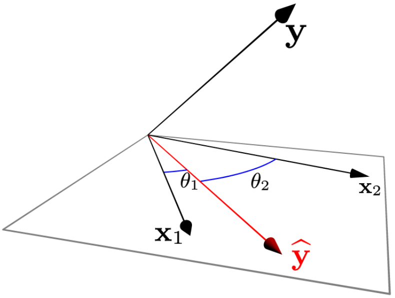
$$y = Xb + e$$

Estimate b as:

$$b = (X^T X)^{-1} X^T y$$

Multiple Regression Loadings

The regression **loadings** should be examined as well as the regression coefficients.



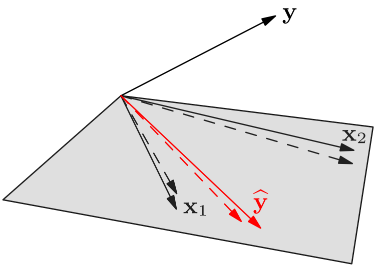
Loadings are given by:

$$\cos\theta_{\vec{x_j},\vec{\hat{y}}} = \frac{\vec{x_j}\cdot\vec{\hat{y}}}{|\vec{x_j}||\vec{\hat{y}}|}$$

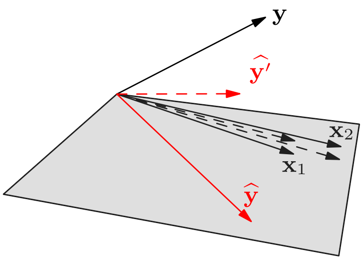
Multiple regression: Cautions and Tips

- Comparing the size of regression coefficients only makes sense if all the predictor variables have the same scale
- The predictor variables (columns of X) must be linearly independent; when they're not the variables are **multicollinear**
- Predictor variables that are **nearly multicollinear** are, perhaps, even more difficult to deal with

Why is near multicollinearity of the predictors a problem?



(a) Non-collinear predictors



(b) Nearly collinear predictors

Figure: When predictors are nearly collinear, small differences in the vectors can result in large differences in the estimated regression.

What can I do if my predictors are (nearly) collinear?

- Drop some of the linearly dependent sets of predictors.
- Replace the linearly dependent predictors with a combined variable.
- Define orthogonal predictors, via linear combinations of the original variables (PC regression approach)
- 'Tweak' the predictor variables so that they're no longer multicollinear (Ridge regression).

Curvilinear Regression

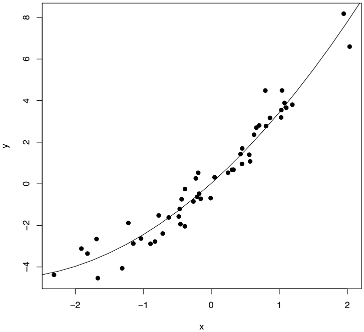
Curvilinear regression using **polynomial models** is simply multiple regression with the x_i replace by powers of x.

$$\hat{y} = b_1 x + b_2 x^2 + \cdots + b_p x^n$$

Note:

- this is still a *linear* regression (linear in the coefficients)
- best applied when a specific hypothesis justifies there use
- generally not higher than quadratic or cubic

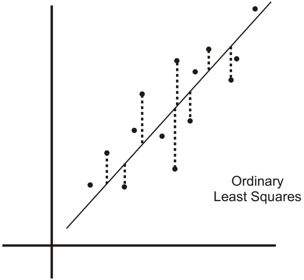
Example of Curvilinear Regression

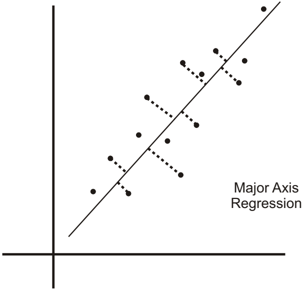


$$y = 3x + 0.5x^2 + e$$

```
lm(formula = y ~ x + I(x^2))
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.02229    0.11651   0.191    0.849
x            2.94001    0.09693  30.331  < 2e-16 ***
I(x^2)       0.47146    0.07685   6.135 1.68e-07 ***
```

Least Squares Regression vs. Major Axis Regression





Vector Geometry of Major Axis Regression

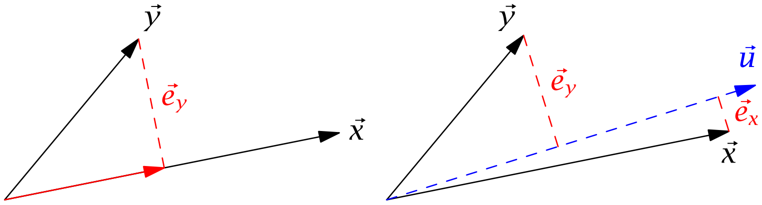


Figure: Vector geometry of ordinary least-squares and major axis regression.

Literate Programming

“Literate programming” is a concept coined by Donald Knuth, a preeminent computer scientist:

- Programs are useless with descriptions.
- Descriptions should be literate, not comments in code or typical reference manuals.
- The code in the descriptions should work.

Literate Programming and Reproducible Research

How literate programming can help to ensure your research is reproducible:

- The steps of your analyses are explicitly described, both as written text and the code and function calls used.
- Analyses can easily checked for correctness and reproduced from your literate code.
- Your literate code can serve as a template for future analyses, saving you time and the trouble of remembering all the gory details.

Tools for literate programming in R

- Sweave – works together with LaTeX to produce output.
- knitr – recent tool developed as a successor to Sweave. More flexible options for input and output; better formatting of figures, etc.

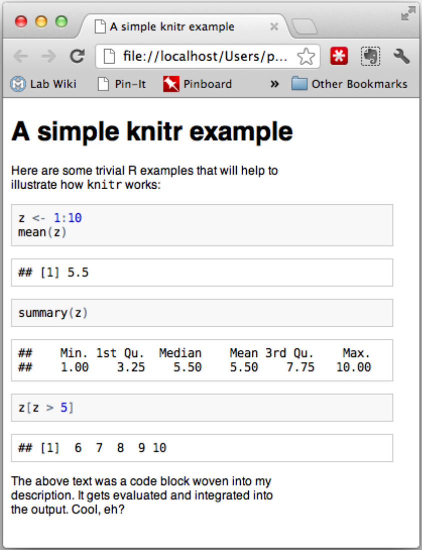
Literate Programming with R Markdown

knitr allows you to use Markdown, a simple markup syntax, to 'weave together' textual descriptions and R code. R code is delimited by so 'code chunks' setoff with three backticks, as illustrated below:

````
# A simple example

Here are some trivial R examples that will help to
illustrate how Sweave works:

```{r}
z <- 1:10
mean(z)
summary(z)
z[z > 5]
```

The above text was a code block woven into my
description. It gets evaluated and integrated into
the output. Cool, eh?
````

knitr output

HTML output produced by knitr for the code on the previous slide:



A simple knitr example

Here are some trivial R examples that will help to illustrate how `knitr` works:

```
z <- 1:10
mean(z)
```

```
## [1] 5.5
```

```
summary(z)
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##    1.00    3.25    5.50    5.50    7.75   10.00
```

```
z[z > 5]
```

```
## [1]  6  7  8  9 10
```

The above text was a code block woven into my description. It gets evaluated and integrated into the output. Cool, eh?

Fancier knitr output

If you go to the trouble of learning to use LaTeX you can generate even nicer output with knitr (code highlighting, better figure formatting):

A knitr example that incorporates graphics is always nice. First, let's generate the data by drawing 1000 observations from the standard normal ($\mu = 0, \sigma = 1$).

```
data <- rnorm(1000)  # 1000 obs. drawn from standard normal
```

Next, we create a summary table:

```
summary(data)

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  -3.470  -0.656   0.004   0.035   0.755   2.930
```

Finally, we create a nice figure in which a density estimate is superimposed on a histogram:

```
hist(data, breaks = 40, freq = F, main = "Hist rnorm(1000)", xlab = "$x$")
lines(density(data), col = "red", lwd = 2)
```