Scientific Computing for Biologists

Multiple Regression

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Variable space view of multiple regression

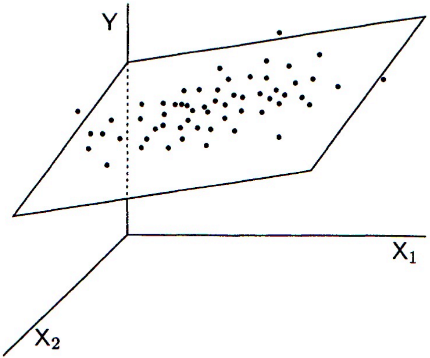
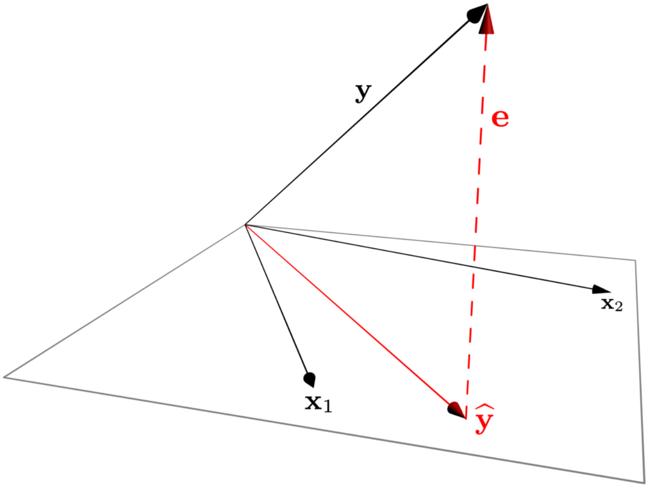


Figure 4.1: *The regression of* Y *onto* X_1 *and* X_2 *as a scatterplot in variable space.*

Subject Space Geometry of Multiple Regression



$$\vec{y} = \vec{\hat{y}} + \vec{e}$$

Multiple Regression

$$\hat{\vec{\boldsymbol{y}}} = a\mathbb{1} + b_1\boldsymbol{X}_1 + b_2\boldsymbol{X}_2 + \cdots + b_p\boldsymbol{X}_p$$

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = a \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} + b_1 \begin{bmatrix} x_{11} \\ x_{21} \\ \vdots \\ x_{n1} \end{bmatrix} + b_2 \begin{bmatrix} x_{12} \\ x_{22} \\ \vdots \\ x_{n2} \end{bmatrix} + \cdots + b_p \begin{bmatrix} x_{1p} \\ x_{2p} \\ \vdots \\ x_{np} \end{bmatrix}$$

$\hat{y}$ is linear combination of the predictor variables

Recall that a *linear combination* of vectors is an equation of the form:

$$z = b_1 \boldsymbol{x}_1 + b_2 \boldsymbol{x}_2 + \cdots + b_p \boldsymbol{x}_p$$

In regression, the vector of fitted values, $\hat{\vec{y}}$, is a linear combination of the predictor variables.

Matrix Representation of Multiple Regression

Let $\vec{y}$ be a vector of values for the outcome variable. Let $\boldsymbol{X}_i$ be explanatory variables. In matrix form:

$$\vec{\boldsymbol{y}} = \boldsymbol{X}\vec{\boldsymbol{b}} + \vec{\boldsymbol{e}}$$

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

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

Estimating the Coefficients for Multiple Regression

$$\vec{\boldsymbol{y}} = \boldsymbol{X}\vec{\boldsymbol{b}} + \vec{\boldsymbol{e}}$$

Estimate $\vec{\boldsymbol{b}}$ as:

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

Matrix Inverses

- If A is a *square matrix* and C is a matrix of the same size where $AC = I$ and $CA = I$ than C is the inverse of A and we denote is A^{-1}.

$$AA^{-1} = A^{-1}A = I$$

- Rules for inverses:
  - Only square matrices are invertible
  - A matrix for which we can find an inverse is called ***invertible*** (non-singular)
  - A matrix for which no inverse exists is ***singular*** (non-invertible)
  - If A and B are both invertible $p \times p$ matrices than $(AB)^{-1} = B^{-1}A^{-1}$ (note change in order).

More facts about Matrix Inverses

- Not every square matrix is invertible
- Every orthogonal matrix is invertible
- Any diagonal matrix, A, where the a_{ii} are non-zero, is invertible

Regression coefficients

$$\vec{\boldsymbol{b}} = \begin{bmatrix} a & b_1 & b_2 & \cdots & b_p \end{bmatrix}^T$$

- The regression coefficients can be thought of as “weightings” of the predictor variables
- Comparing the magnitude of regression coefficients only makes sense if all the predictor variables have the same scale
- If predictor variables have different scales, then can can first standardize the variables (subtract means and divide by variances), before fitting regression to get standardized regression coefficients.
- Alternately, calculate standardized regression coefficients as:

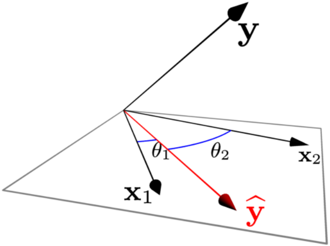
$$b'_j = \frac{|\vec{\boldsymbol{x}}_j|}{|\vec{\boldsymbol{y}}|} b_j$$

Regression loadings

The correlation between each predictor variable, $\boldsymbol{x}_j$ and the prediction, $\vec{\hat{y}}$, is given by the angle between them:

$$\cos\theta_{\overrightarrow{x_j},\vec{\hat{y}}} = \frac{\overrightarrow{\boldsymbol{x}_j} \cdot \vec{\hat{\boldsymbol{y}}}}{|\overrightarrow{\boldsymbol{x}_j}||\vec{\hat{\boldsymbol{y}}}|}$$

These are sometimes called “loadings” and should be examined in combination with the regression coefficients to understand the model implied by the multiple regression.



Coefficient of determination

The coefficient of determination, R^2, is the standard measure of the fraction of variation 'explained' by the regression model.
This is equivalent to the cosine of angle between the outcome vector and the predicted outcome vector, squared.

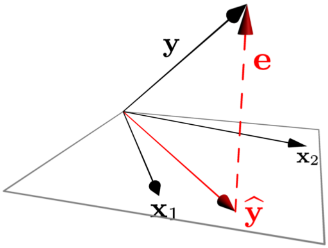
$$R^2 = (\cos\theta_{\vec{y},\vec{\hat{y}}})^2 = \frac{|\vec{\hat{\boldsymbol{y}}}|^2}{|\vec{\boldsymbol{y}}|^2} = \frac{\vec{\hat{\boldsymbol{y}}} \cdot \vec{\hat{\boldsymbol{y}}}}{\vec{\boldsymbol{y}} \cdot \vec{\boldsymbol{y}}}$$

Note that the vector formulation above assumes mean-centered $\vec{\boldsymbol{y}}$ and $\vec{\hat{\boldsymbol{y}}}$.

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.



The prediction, $\hat{\vec{y}}$ is the closest vector to $\vec{y}$ in the space spanned by the predictor variables, $\boldsymbol{X}$.

The predictor variables must be linearly independent

To solve the multiple regression equation, the predictor variables, $\boldsymbol{X}$, must be linearly independent.

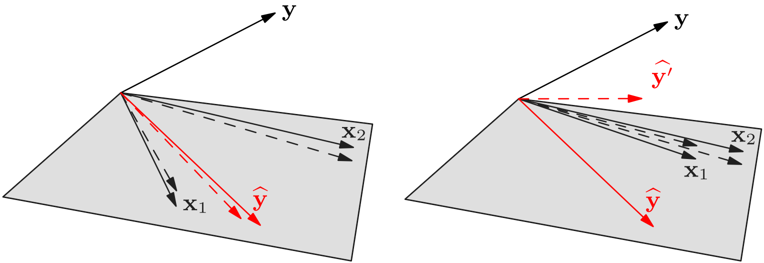
- A list of vectors, $\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_p$, is said the be ***linearly dependent*** if there is a non-trivial combination of them which is equal to the zero vector.

$$b_1\boldsymbol{x}_1 + b_2\boldsymbol{x}_2 + \cdots + b_p\boldsymbol{x}_p = 0$$

- When a set of vectors are linearly dependent we also called them ***multicollinear***
- A list of vectors that are *not* linearly dependent are said to be ***linearly independent***
- If a matrix is invertible than it's columns form a linearly independent list of vectors!

Near multicollinearity of the predictors leads to unstable regression solutions

Predictor variables that are **nearly multicollinear** are, perhaps, even more difficult to deal with:



(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

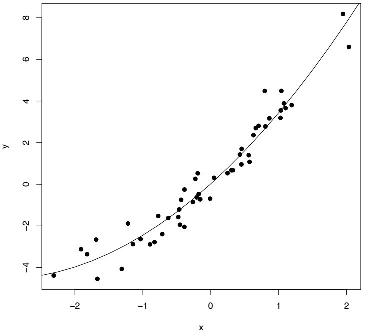
Curvilinear regression using **polynomial models** is simply multiple regression with the x_i replace by powers of x.

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

Note:

- this is still a *linear* regression (linear in the coefficients)
- best applied when a specific hypothesis justifies their 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 ***
```