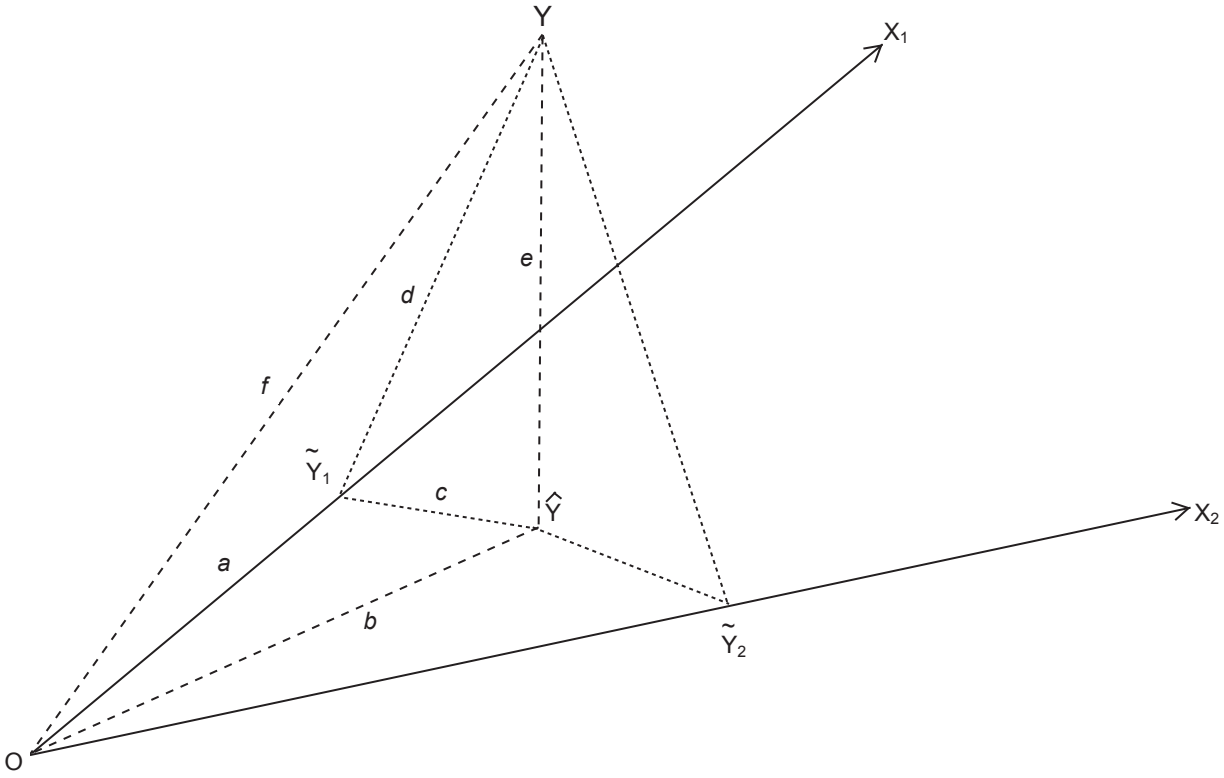
MATH 523: THE GEOMETRY OF MULTICOLLINEARITY AND SUMS OF SQUARES

Consider a two covariate linear model with (collections of) covariates X_1 and X_2. Let

- $\widetilde{Y}_1 = X_1\widetilde{\beta}_1$ be the least-squares fit using only X_1.
- $\widetilde{Y}_2 = X_2\widetilde{\beta}_2$ be the least-squares fit using only X_2.
- $\widehat{Y} = X_1\widehat{\beta}_1 + X_2\widehat{\beta}_2$ be the least-squares fit using both X_1 and X_2.



so that, for example

Vector	$O\widetilde{Y}_1$	$O\widehat{Y}$	$\widetilde{Y}_1\widehat{Y}$	$\widetilde{Y}_1Y$	$\widehat{Y}Y$	OY
Length	a	b	c	d	e	f

By previous orthogonality results,

(i) $\widetilde{Y}_1$ is the projection of Y onto the X_1 subspace, hence the angle $O\widetilde{Y}_1Y$ is a right angle, so

$$||O\widetilde{Y}_1||^2 + ||\widetilde{Y}_1Y||^2 = ||OY||^2$$

or $a^2 + d^2 = f^2$.

(ii) $\widehat{Y}$ is the projection of Y onto the (X_1, X_2) subspace, hence the angle $O\widehat{Y}Y$ is a right angle, so

$$||O\widehat{Y}||^2 + ||\widehat{Y}Y||^2 = ||OY||^2$$

or $b^2 + e^2 = f^2$.

However, $\widetilde{Y}_1\widehat{Y}Y$ is also a right angle, so $c^2 + e^2 = d^2$. Hence we must have also that $a^2 + c^2 = b^2$, and can deduce that $O\widetilde{Y}_1\widehat{Y}$ is also a right angle. Thus $\widetilde{Y}_1$ is the projection of $\widehat{Y}$ onto the X_1 space. By similar arguments, $\widetilde{Y}_2$ is the projection of $\widehat{Y}$ onto the X_2 space.

Two sequential model fitting strategies are possible:

(I) Fit X_1, then fit X_2 to the residual after fitting X_1. This yields the sum of squares decomposition

$$\begin{aligned} ||OY||^2 &= ||O\widetilde{Y}_1||^2 + ||\widetilde{Y}_1\widehat{Y}||^2 + ||\widehat{Y}Y||^2 \\ Y^\mathsf{T}Y &= \widetilde{\beta}_1^\mathsf{T}X_1^\mathsf{T}X_1\widetilde{\beta}_1 + (X_1\widehat{\beta}_1 + X_2\widehat{\beta}_2 - X_1\widetilde{\beta}_1)^\mathsf{T}(X_1\widehat{\beta}_1 + X_2\widehat{\beta}_2 - X_1\widetilde{\beta}_1) \\ &\quad +(Y - X_1\widehat{\beta}_1 - X_2\widehat{\beta}_2)^\mathsf{T}(Y - X_1\widehat{\beta}_1 - X_2\widehat{\beta}_2) \end{aligned}$$

(II) Fit X_2, then fit X_1 to the residual after fitting X_2. This yields the sum of squares decomposition

$$\begin{aligned} ||OY||^2 &= ||O\widetilde{Y}_2||^2 + ||\widetilde{Y}_2\widehat{Y}||^2 + ||\widehat{Y}Y||^2 \\ Y^\mathsf{T}Y &= \widetilde{\beta}_2^\mathsf{T}X_2^\mathsf{T}X_2\widetilde{\beta}_2 + (X_1\widehat{\beta}_1 + X_2\widehat{\beta}_2 - X_2\widetilde{\beta}_2)^\mathsf{T}(X_1\widehat{\beta}_1 + X_2\widehat{\beta}_2 - X_2\widetilde{\beta}_2) \\ &\quad +(Y - X_1\widehat{\beta}_1 - X_2\widehat{\beta}_2)^\mathsf{T}(Y - X_1\widehat{\beta}_1 - X_2\widehat{\beta}_2) \end{aligned}$$

The terms $||OY||^2$ and $||\widehat{Y}Y||^2$ are common to both expressions, and independent of the strategy. Thus, in the usual terminology, we have two equivalent expressions for the ***fitted sum of squares***

$$||O\widetilde{Y}_1||^2 + ||\widetilde{Y}_1\widehat{Y}||^2 = ||O\widetilde{Y}_2||^2 + ||\widetilde{Y}_2\widehat{Y}||^2$$

Using the standard formulae, we have that if $\mathbf{X} = [X_1^\mathsf{T},\ X_2^\mathsf{T}]^\mathsf{T}$, then

$$\mathbf{X}^\mathsf{T}\mathbf{X} = \begin{bmatrix} X_1^\mathsf{T}X_1 & X_1^\mathsf{T}X_2 \\ X_2^\mathsf{T}X_1 & X_2^\mathsf{T}X_2 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \qquad \therefore \qquad (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1} = \begin{bmatrix} A & B \\ B^\mathsf{T} & C \end{bmatrix}$$

say, where

$$A = (S_{11} - S_{12}S_{22}^{-1})^{-1} \qquad B = -S_{11}S_{12}(S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1} \qquad C = (S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1}$$

Therefore, for the model with both covariates, we have

$$\widehat{\beta} = \begin{bmatrix} \widehat{\beta}_1 \\ \widehat{\beta}_2 \end{bmatrix} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}Y = \begin{bmatrix} AX_1^\mathsf{T}Y + BX_2^\mathsf{T}Y \\ B^\mathsf{T}X_1^\mathsf{T}Y + CX_2^\mathsf{T}Y \end{bmatrix}$$

so that

$$\begin{aligned} \widehat{\beta}_1 &= (X_1^\mathsf{T}X_1 - (X_1^\mathsf{T}X_2)(X_2^\mathsf{T}X_2)^{-1}(X_2^\mathsf{T}X_1))^{-1}X_1^\mathsf{T}Y \\ &\quad - \left\{(X_1^\mathsf{T}X_1)^{-1}(X_1^\mathsf{T}X_2)\left(X_2^\mathsf{T}X_2 - (X_2^\mathsf{T}X_1)(X_1^\mathsf{T}X_1)^{-1}(X_1^\mathsf{T}X_2)\right)\right\}X_2^\mathsf{T}Y \end{aligned}$$

whereas for the model with just X_1

$$\widetilde{\beta}_1 = (X_1^\mathsf{T}X_1)^{-1}X_1^\mathsf{T}Y.$$

Therefore if $X_1^\mathsf{T}X_2 \neq 0$, $\widehat{\beta}_1 \neq \widetilde{\beta}_1$. If $X_1^\mathsf{T}X_2 = 0$, so that X_1 and X_2 are orthogonal, then in the figure, the angle

$$\widetilde{Y}_1O\widetilde{Y}_2$$

is also a right angle.