

The Geometry of Vector Spaces

$\mathbf{x} \in E^N$: vector $\mathbf{x}$ belongs to an N -dimensional Euclidean space.

The **Inner product** of vectors $\mathbf{x}$ and $\mathbf{y} \in E^N$ is

$$\langle \mathbf{x}, \mathbf{y} \rangle \equiv \mathbf{x}^\top \mathbf{y}. \quad (1)$$

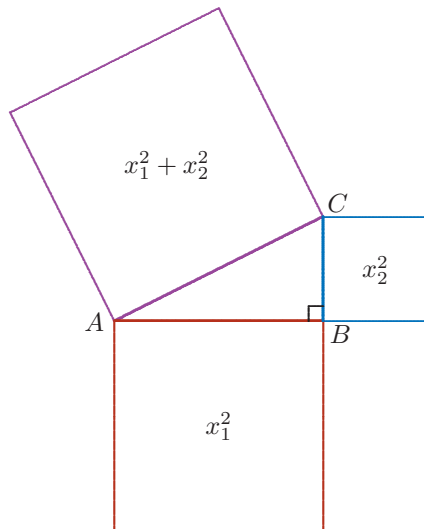
The **length** or **norm** of a vector $\mathbf{x}$ in E^N is

$$\|\mathbf{x}\| \equiv (\mathbf{x}^\top \mathbf{x})^{1/2} = \left(\sum_{i=1}^N x_i^2 \right)^{1/2}. \quad (2)$$

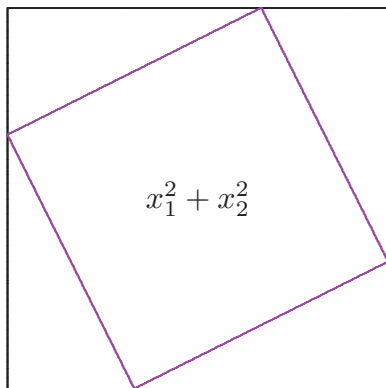
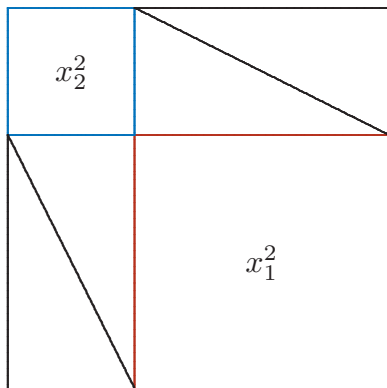
A vector $\mathbf{x}$ in E^2 has coordinates x_1 and x_2 .

Pythagoras' Theorem tells us that the length of the vector $\mathbf{x}$, the hypotenuse of a right-angled triangle, is $(x_1^2 + x_2^2)^{1/2}$.

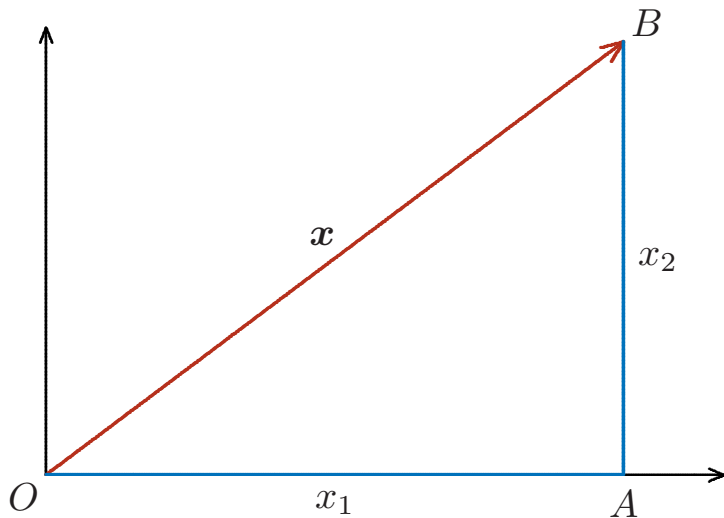
Pythagoras' Theorem



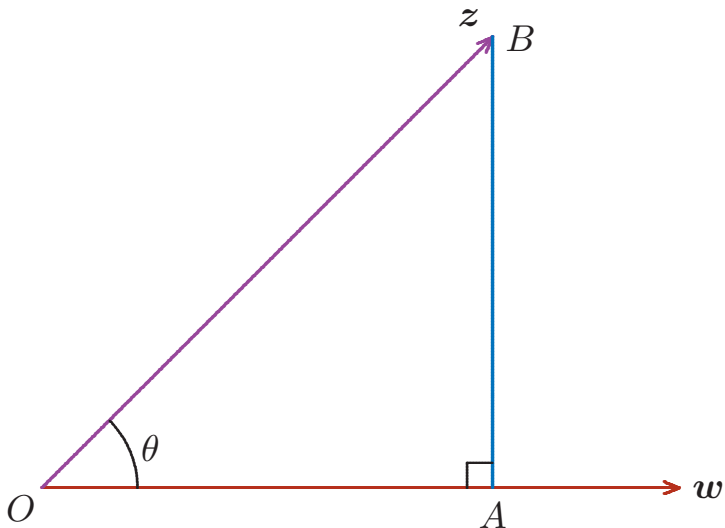
Proof of Pythagoras' Theorem



A Vector x in E^2



The Angle Between Two Vectors



Let w and z be vectors of length 1, and let θ denote the angle between them. This is illustrated in the figure just shown.

w has coordinates $(1, 0)$ and is represented by a horizontal line of length 1. Since z is also of length 1, $\|z\| = 1$.

Because

$$\|z\|^2 = \cos^2 \theta + \sin^2 \theta = 1, \quad (3)$$

the coordinates of z must be $(\cos \theta, \sin \theta)$.

The scalar product of w and z is

$$\langle w, z \rangle = w^\top z = w_1 z_1 + w_2 z_2 = z_1 = \cos \theta, \quad (4)$$

because w has coordinates $(1, 0)$.

More generally, if $x = \alpha w$ and $y = \gamma z$, for positive scalars α and γ , then $\|x\| = \alpha$ and $\|y\| = \gamma$. Thus

$$\langle x, y \rangle = x^\top y = \alpha \gamma w^\top z = \alpha \gamma \langle w, z \rangle. \quad (5)$$

Because x is parallel to w , and y is parallel to z , the angle between x and y is the same as that between w and z , namely θ . Therefore,

$$\langle x, y \rangle = \|x\| \|y\| \cos \theta. \quad (6)$$

The inner product of any two vectors x and y is the product of their lengths times the cosine of the angle between them.

- $\cos \theta$ varies between -1 and 1 .
- $\cos 0 = 1$, $\cos \pi/2 = 0$, and $\cos \pi = -1$.
- $\cos \theta$ is 1 for vectors that are parallel.
- $\cos \theta$ is 0 for vectors that are at right angles to each other.
- $\cos \theta$ is -1 for vectors that point in directly opposite directions.
- If x and y form a right angle, then $\cos \theta = 0$, and $\langle x, y \rangle = 0$.
- If $\langle x, y \rangle = 0$, then $\cos \theta = 0$ unless x or y is a zero vector. Except in that special case, $\theta = \pi/2$ when $\langle x, y \rangle = 0$.

An implication of (6) is the **Cauchy-Schwartz inequality**,

$$|\mathbf{x}^\top \mathbf{y}| \leq \|\mathbf{x}\| \|\mathbf{y}\|. \quad (7)$$

This becomes an equality only when $\mathbf{x}$ and $\mathbf{y}$ are parallel, so that $|\cos \theta| = 1$.

Vectors that are at right angles are said to be **orthogonal** or **perpendicular**.

Now consider the regression model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{u}. \quad (8)$$

Here $\mathbf{y}$ and each column of $\mathbf{X}$ can be thought of as vectors in E^N .

Denote the k columns of $\mathbf{X}$ (assumed to have full rank) as $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k$.

These k **basis vectors** are said to **span** a k -dimensional **subspace**.

The subspace they span may be denoted $\mathcal{S}(\mathbf{X})$ or $\mathcal{S}(\mathbf{x}_1, \dots, \mathbf{x}_k)$.

- $\mathcal{S}(x_1, \dots, x_k)$ consists of every vector that can be formed as a **linear combination** of the $x_i, i = 1, \dots, k$. Formally,

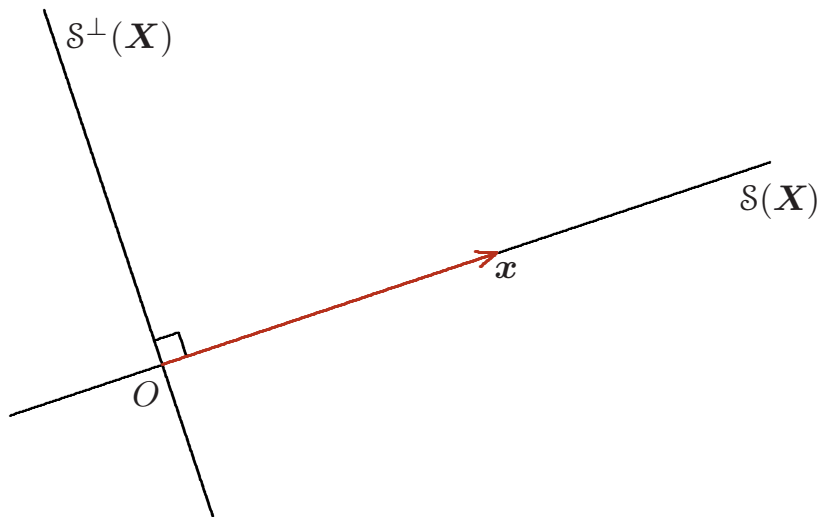
$$\mathcal{S}(x_1, \dots, x_k) \equiv \left\{ z \in E^N \mid z = \sum_{i=1}^k b_i x_i, \quad b_i \in \mathbb{R} \right\}. \quad (9)$$

- $\mathcal{S}(X)$ is called the subspace spanned by the x_i , or the **column space** of X , or the **span** of X , or the span of the x_i .
- For every dataset $[y, X]$, both y and every column of X lie in E^N , and X defines a k -dimensional subspace, $\mathcal{S}(X)$.
- The **orthogonal complement** of $\mathcal{S}(X)$ in E^N , denoted $\mathcal{S}^\perp(X)$, is the set of all vectors w in E^N that are orthogonal to everything in $\mathcal{S}(X)$:

$$\mathcal{S}^\perp(X) \equiv \left\{ w \in E^N \mid w^\top z = 0 \text{ for all } z \in \mathcal{S}(X) \right\}. \quad (10)$$

If dimension of $\mathcal{S}(X)$ is k , then dimension of $\mathcal{S}^\perp(X)$ is $N - k$.

The Spaces $\mathcal{S}(X)$ and $\mathcal{S}^\perp(X)$



- If X does not have full rank k , then the dimension of $\mathcal{S}(X)$ is less than k , and the dimension of $\mathcal{S}^\perp(X)$ is greater than $N - k$.
- When X has full rank, the columns of X are **linearly independent**.
- The vectors $\mathbf{x}_1$ through $\mathbf{x}_k$ are said to be **linearly dependent** if there is a vector $\mathbf{x}_j$, $1 \leq j \leq k$, and coefficients c_i such that

$$\mathbf{x}_j = \sum_{i \neq j} c_i \mathbf{x}_i. \quad (11)$$

- Equivalently, there exist coefficients b_i , at least one of which is nonzero, such that

$$\sum_{i=1}^k b_i \mathbf{x}_i = \mathbf{0}, \quad \text{or} \quad X\mathbf{b} = \mathbf{0}. \quad (12)$$

- If $\mathbf{x}_j = \mathbf{0}$, then (12) is satisfied if we make b_j nonzero and set $b_i = 0$ for all $i \neq j$. So linear independence rules out $\mathbf{x}_j = \mathbf{0}$ for any j .

- If the columns of X are linearly dependent, there must exist a nonzero vector $\mathbf{b}$ such that $X\mathbf{b} = \mathbf{0}$.
- Premultiplying the second equation in (12) by $X^\top$ yields

$$X^\top X\mathbf{b} = \mathbf{0}. \quad (13)$$

But if $X^\top X$ is invertible, there exists $(X^\top X)^{-1}$ such that $(X^\top X)^{-1}(X^\top X) = \mathbf{I}$, the $k \times k$ identity matrix.

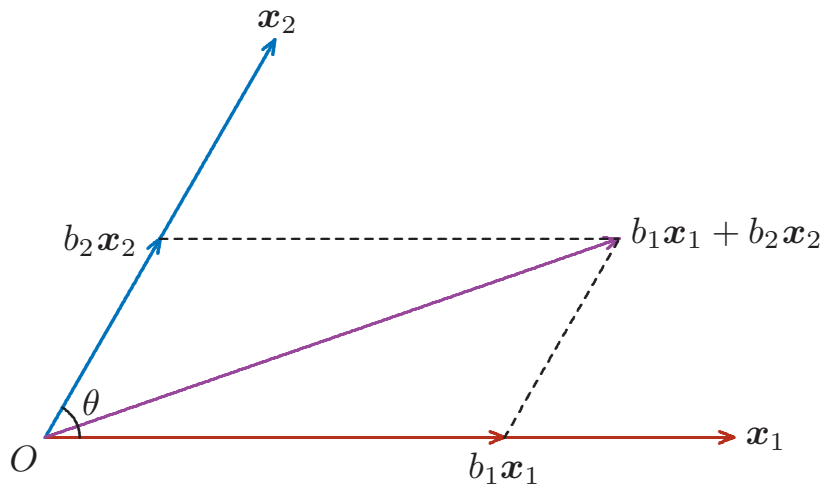
- Thus (13) implies that

$$\mathbf{b} = \mathbf{I}\mathbf{b} = (X^\top X)^{-1}X^\top X\mathbf{b} = \mathbf{0}. \quad (14)$$

But this is a contradiction, since we have assumed that $\mathbf{b} \neq \mathbf{0}$.

- We conclude that $X^\top X$ cannot have an inverse if the columns of X are linearly dependent.

A Two-Dimensional Subspace



When the dimension of $\mathcal{S}(X)$ is $k' < k$, $\mathcal{S}(X)$ must be identical to $\mathcal{S}(X')$, where X' is an $N \times k'$ matrix consisting of any k' linearly independent columns of X . Consider

$$X = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 4 & 0 \\ 1 & 0 & 1 \\ 1 & 4 & 0 \\ 1 & 0 & 1 \end{bmatrix}. \quad (15)$$

The columns of this matrix are not linearly independent, since $x_1 = \frac{1}{4}x_2 + x_3$. However, any two of the columns are linearly independent. Therefore,

$$\mathcal{S}(X) = \mathcal{S}(x_1, x_2) = \mathcal{S}(x_1, x_3) = \mathcal{S}(x_2, x_3). \quad (16)$$

Henceforth, we will generally assume that the columns of any regressor matrix X are linearly independent.

The Geometry of OLS Estimation

When $\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_k]$, then

$$\mathbf{X}\boldsymbol{\beta} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_k] \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix} = \mathbf{x}_1\beta_1 + \mathbf{x}_2\beta_2 + \cdots + \mathbf{x}_k\beta_k = \sum_{i=1}^k \beta_i \mathbf{x}_i. \quad (17)$$

The moment conditions are

$$\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) = \mathbf{0}. \quad (18)$$

This tells us that the **residual vector** $\hat{\mathbf{u}} \equiv \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}$ is orthogonal to every regressor.

Thus $\hat{\mathbf{u}}$ must lie in $\mathcal{S}^\perp(\mathbf{X})$.

(18) implies that $\hat{\mathbf{u}}$ is orthogonal to *every* vector in $\mathcal{S}(\mathbf{X})$. Since $\mathbf{X}^\top \hat{\mathbf{u}} = \mathbf{0}$, then for every $\boldsymbol{\beta}$

$$(\mathbf{X}\boldsymbol{\beta})^\top \hat{\mathbf{u}} = \boldsymbol{\beta}^\top \mathbf{X}^\top \hat{\mathbf{u}} = \mathbf{0}. \quad (19)$$

The vector $\mathbf{X}\hat{\boldsymbol{\beta}}$ is referred to as the vector of **fitted values**. Clearly, it lies in $\mathcal{S}(\mathbf{X})$, and, consequently, it must be orthogonal to $\hat{\mathbf{u}}$.

By Pythagoras' Theorem,

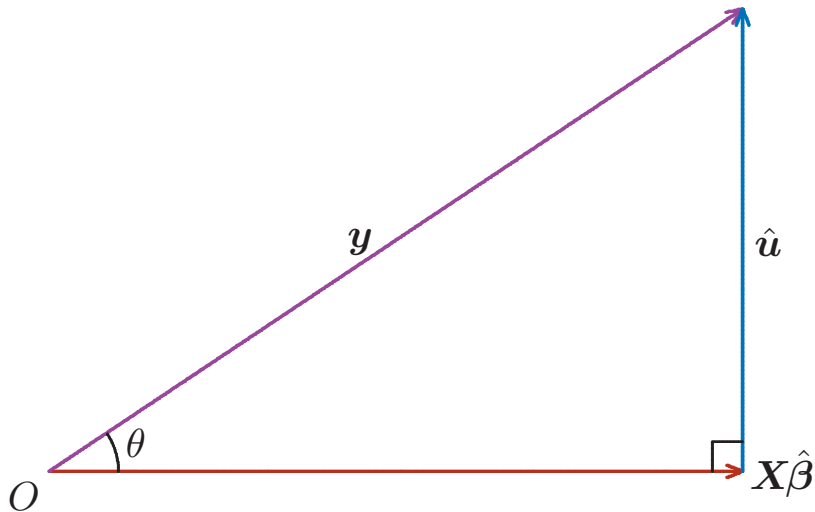
$$\|\mathbf{y}\|^2 = \|\mathbf{X}\hat{\boldsymbol{\beta}}\|^2 + \|\hat{\mathbf{u}}\|^2. \quad (20)$$

If we write out the squared norms as scalar products, this becomes

$$\mathbf{y}^\top \mathbf{y} = \hat{\boldsymbol{\beta}}^\top \mathbf{X}^\top \mathbf{X} \hat{\boldsymbol{\beta}} + (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}). \quad (21)$$

The **total sum of squares**, or **TSS**, is equal to the **explained sum of squares**, or **ESS**, plus the **sum of squared residuals**, or **SSR**.

Residuals and Fitted Values



Projections and Projection Matrices

A **projection** maps each point of E^N into a point in a subspace of E^N .

An **orthogonal projection** maps any point into the point of the subspace that is closest to it.

An orthogonal projection of any vector on to a given subspace can be performed by premultiplying the vector by a suitable **projection matrix**. For an N -vector, it is an $N \times N$ matrix.

The projection matrices that yield fitted values and residuals are

$$P_X = X(X^\top X)^{-1}X^\top \quad \text{and} \quad (22)$$

$$M_X = I - P_X = I - X(X^\top X)^{-1}X^\top, \quad (23)$$

where I is the $N \times N$ identity matrix.

Notice that P_X and M_X are both symmetric matrices.

The **invariant subspace** or **image** of P_X is $\mathcal{S}(X)$.

Since

$$\hat{\beta} = (X^\top X)^{-1} X^\top y, \quad (24)$$

then

$$X\hat{\beta} = X(X^\top X)^{-1} X^\top y = P_X y, \quad (25)$$

and

$$P_X Xb = Xb. \quad (26)$$

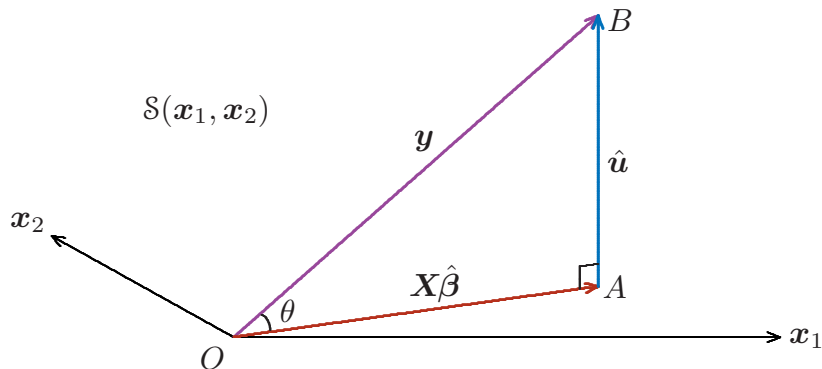
Thus P_X maps any vector in $\mathcal{S}(X)$ into itself.

Similarly, when M_X is applied to y , it yields the vector of residuals

$$M_X y = (I - X(X^\top X)^{-1} X^\top) y = y - P_X y = y - X\hat{\beta} = \hat{u}. \quad (27)$$

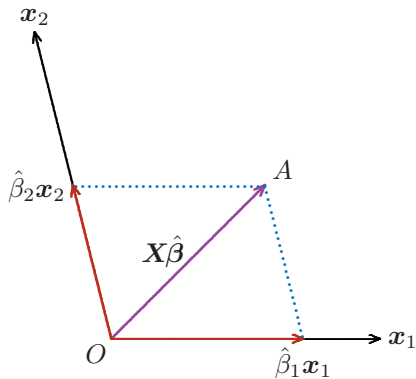
The image of M_X is $\mathcal{S}^\perp(X)$, which is the orthogonal complement of the image of P_X .

Linear Regression in Three Dimensions

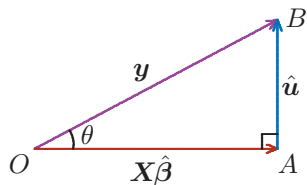


(a) y projected on two regressors

Linear Regression in Three Dimensions



(b) The span $\mathcal{S}(x_1, x_2)$ of the regressors



(c) The vertical plane through y

The equality

$$(M_X \mathbf{y})^\top \mathbf{X} = \mathbf{y}^\top M_X \mathbf{X} \quad (28)$$

relies on the symmetry of M_X . Then, from (23), we have

$$M_X \mathbf{X} = (\mathbf{I} - P_X) \mathbf{X} = \mathbf{X} - \mathbf{X} = \mathbf{O}, \quad (29)$$

For any matrix to represent a projection, it must be **idempotent**. When multiplied by itself, an idempotent matrix yields itself again. Thus,

$$P_X P_X = P_X \quad \text{and} \quad M_X M_X = M_X. \quad (30)$$

This must be the case, because $P_X \mathbf{a} = P_X P_X \mathbf{a}$ for any vector $\mathbf{a}$. Similarly, $M_X \mathbf{a} = M_X M_X \mathbf{a}$ for any vector $\mathbf{a}$.

Geometrically, P_X takes $\mathbf{a}$ to the closest point in $\mathcal{S}(X)$. Since the vector $P_X \mathbf{a}$ is already at that point, $P_X P_X \mathbf{a}$ has nowhere else to go.

Geometrically, M_X takes $\mathbf{a}$ to the closest point in $\mathcal{S}^\perp(X)$.

Since, from (23),

$$P_X + M_X = I, \quad (31)$$

any vector $\mathbf{y} \in E^N$ is equal to $P_X \mathbf{y} + M_X \mathbf{y}$.

The pair of projections P_X and M_X are said to be **complementary projections**.

The projection matrices P_X and M_X define an **orthogonal decomposition** of E^N , because $M_X \mathbf{y}$ and $P_X \mathbf{y}$ lie in two orthogonal subspaces.

Evidently,

$$P_X M_X = \mathbf{O}. \quad (32)$$

We may say that P_X and M_X **annihilate** each other.

Now consider any vectors $\mathbf{z} \in \mathcal{S}(X)$ and $\mathbf{w} \in \mathcal{S}^\perp(X)$.

Since $\mathbf{z} = \mathbf{P}_X \mathbf{z}$ and $\mathbf{w} = \mathbf{M}_X \mathbf{w}$,

$$\mathbf{z}^\top \mathbf{w} = (\mathbf{P}_X^\top \mathbf{z})^\top \mathbf{M}_X \mathbf{w} \quad (33)$$

$$= \mathbf{z}^\top \mathbf{P}_X \mathbf{M}_X \mathbf{w} = 0. \quad (34)$$

$\mathbf{M}_X$ annihilates all points that lie in $\mathcal{S}(X)$, and $\mathbf{P}_X$ likewise annihilates all points that lie in $\mathcal{S}^\perp(X)$.

An orthogonal decomposition $\mathbf{y} = \mathbf{P}_X \mathbf{y} + \mathbf{M}_X \mathbf{y}$ can be represented by a right-angled triangle, with $\mathbf{y}$ as the hypotenuse and $\mathbf{P}_X \mathbf{y}$ and $\mathbf{M}_X \mathbf{y}$ as the other two sides.

The relationship between TSS, ESS, and SSR given in (21) is just Pythagoras' Theorem:

$$\|\mathbf{y}\|^2 = \|\mathbf{P}_X \mathbf{y}\|^2 + \|\mathbf{M}_X \mathbf{y}\|^2. \quad (35)$$

Because the hypotenuse of a right-angled triangle is longer than either of the other two sides, $\text{ESS} \leq \text{TSS}$, and $\text{SSR} \leq \text{TSS}$.

Of course, projection matrices may be associated with any subspaces, not just $\mathcal{S}(X)$ and $\mathcal{S}^\perp(X)$. Here are some examples:

- P_Z is the matrix that projects orthogonally on to $\mathcal{S}(Z)$;
- $M_{X,W}$ is the matrix that projects orthogonally off $\mathcal{S}(X, W)$, or on to $\mathcal{S}^\perp(X, W)$.
- $P_{[X_1 \ X_2]}$ is the matrix that projects orthogonally on to $\mathcal{S}(X) = \mathcal{S}([X_1 \ X_2]) = \mathcal{S}(X_1, X_2)$, where $X = [X_1 \ X_2]$.
- $P_{X_1} = P_1$ is the matrix that projects orthogonally on to $\mathcal{S}(X_1)$.
- $M_{P_Z X}$ is the matrix that projects orthogonally on to $\mathcal{S}^\perp(P_Z X)$.

Note that $P_X = P_{[X_1 \ X_2]} = P_{X_1} + P_{M_1 X_2}$.

We can add the two projection matrices here to obtain another projection matrix, because everything in $\mathcal{S}(M_1 X_2)$ is orthogonal to everything in $\mathcal{S}(X_1)$.

In general, however, the sum of two projection matrices is not a projection matrix.

Let A be partitioned by its columns, which may be denoted $\mathbf{a}_i$, $i = 1, \dots, k$:

$$XA = X \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_k \end{bmatrix} = \begin{bmatrix} X\mathbf{a}_1 & X\mathbf{a}_2 & \cdots & X\mathbf{a}_k \end{bmatrix}. \quad (36)$$

Each block here takes the form $X\mathbf{a}_i$, which is a linear combination of the columns of X .

Thus any element of $\mathcal{S}(XA)$ must also be an element of $\mathcal{S}(X)$. But any element of $\mathcal{S}(X)$ is also an element of $\mathcal{S}(XA)$.

Any element of $\mathcal{S}(X)$ can be written as $X\boldsymbol{\beta}$ for some $\boldsymbol{\beta} \in \mathbb{R}^k$. Since A is nonsingular, and thus invertible,

$$X\boldsymbol{\beta} = XAA^{-1}\boldsymbol{\beta} = (XA)(A^{-1}\boldsymbol{\beta}). \quad (37)$$

Since every element of $\mathcal{S}(XA)$ belongs to $\mathcal{S}(X)$, and every element of $\mathcal{S}(X)$ belongs to $\mathcal{S}(XA)$, these two subspaces must be identical.

The orthogonal projections P_X and P_{XA} are the same:

$$P_{XA} = XA(A^\top X^\top XA)^{-1}A^\top X^\top \quad (38)$$

$$= XAA^{-1}(X^\top X)^{-1}(A^\top)^{-1}A^\top X^\top \quad (39)$$

$$= X(X^\top X)^{-1}X^\top = P_X. \quad (40)$$

The fitted values and residuals depend on X only through P_X and M_X , so they too must be invariant to any nonsingular linear transformation of the columns of X .

Consider a temperature variable T in Celsius or F in Fahrenheit:

$$F = 32\iota + \frac{9}{5}T. \quad (41)$$

If the constant is included in the transformation, then

$$\begin{bmatrix} \iota & F \end{bmatrix} = \begin{bmatrix} \iota & T \end{bmatrix} \begin{bmatrix} 1 & 32 \\ 0 & 9/5 \end{bmatrix}. \quad (42)$$

Residuals and fitted values are unaffected.

Suppose the constant term and slope coefficient in the regression using Celsius are β_1 and β_2 .

Similarly, the constant term and slope coefficient in the regression using Fahrenheit are α_1 and α_2 .

Then

$$\beta_1 = \alpha_1 + 32\alpha_2 \quad \text{and} \quad \beta_2 = \frac{9}{5}\alpha_2. \quad (43)$$

It is often good to rescale regressors to ensure that:

- Coefficient estimates are of similar magnitude;
- The eigenvalues of $\mathbf{X}^\top \mathbf{X}$ do not differ so much that OLS estimates may be numerically unreliable.

We may redefine regressors so that the coefficients are meaningful:

$$\begin{aligned} \mathbf{y} &= \beta_1 + \beta_2 \mathbf{x}_2 + \beta_3 \mathbf{x}_3 + \mathbf{u} \\ &= \beta_1 + \beta_2 (\mathbf{x}_2 + \mathbf{x}_3) + (\beta_3 - \beta_2) \mathbf{x}_3 + \mathbf{u}. \end{aligned} \quad (44)$$

The coefficient on $\mathbf{x}_3$ is now $\beta_3 - \beta_2$.