

Scientific Computing for Biologists

Data as Vectors

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Overview of Lecture

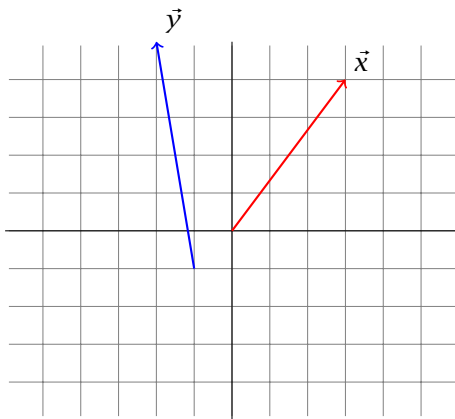
- Vector Geometry
 - Vectors are directed line segments
 - Vector length
- Vector Arithmetic
 - Addition, subtraction
 - Scalar multiplication
 - Linear combinations of vectors
 - Dot product and projection
- Vector representations of multivariate data
 - Variable space/Subject space representations
 - Mean as projection in subject space
 - Bivariate regression in geometric terms
 - Difference in group means as a regression problem

Hands-on Session

- Vector operations in R
- Writing functions in R
- Visualizing bivariate relationships in R
- Linear regression in R

Vector Geometry

Vectors are directed line segments.

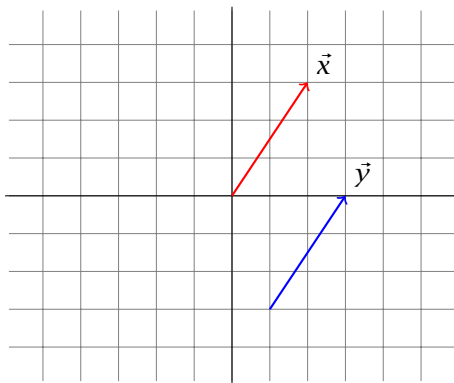


All of the figures and algebraic formulas I show you apply to n -dimensional vectors.

Vector Geometry

Vectors have direction and length:

$$\vec{x} = [x_1, x_2]' = [2, 3]'; |\vec{x}| = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$$

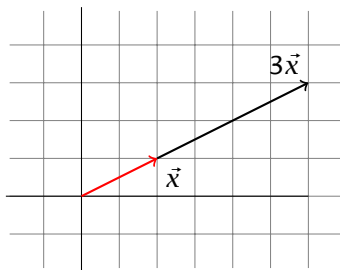


Often starting point is ignored, in which case $\vec{x} = \vec{y}$.

Scalar Multiplication of a Vector

Let k be a scalar.

$$k\vec{x} = \begin{bmatrix} kx_1 \\ kx_2 \\ \vdots \\ kx_n \end{bmatrix}$$

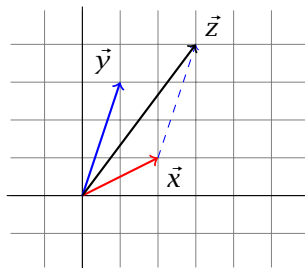


$$\vec{x} = [2, 1]'; \quad 3\vec{x} = [6, 3]'.$$

Vector Addition

Let $\vec{x} = [2, 1]'$; $\vec{y} = [1, 3]'$

$$\vec{z} = \vec{x} + \vec{y} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{bmatrix}$$

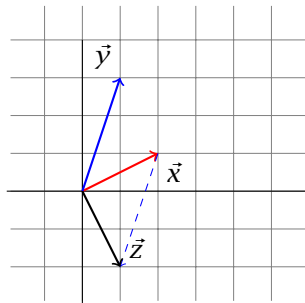


Addition follows the 'head-to-tail' rule.

Vector Subtraction

Let $\vec{x} = [2, 1]'$; $\vec{y} = [1, 3]'$

$$\vec{z} = \vec{x} - \vec{y} = \begin{bmatrix} x_1 - y_1 \\ x_2 - y_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

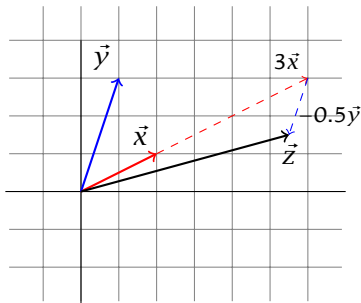


Follow the addition rule for $-1\vec{y}$.

Linear Combinations of Vectors

A linear combination of vectors is of the form $z = b_1\vec{x} + b_2\vec{y}$

$$\vec{z} = 3\vec{x} - 0.5\vec{y} = 3 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - 0.5 \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

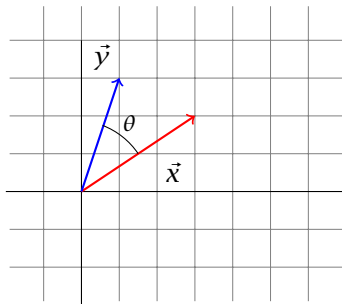


Dot Product

The dot (inner) product of two vectors, $\vec{x} \cdot \vec{y}$ is a scalar.

$$\begin{aligned}\vec{x} \cdot \vec{y} &= x_1y_1 + x_2y_2 + \cdots + x_ny_n \\ &= |\vec{x}||\vec{y}| \cos \theta\end{aligned}$$

where θ is the angle (in radians) between \vec{x} and \vec{y}



$$\vec{x} = [3, 2]', \vec{y} = [1, 3]'; \vec{x} \cdot \vec{y} = \sqrt{13}\sqrt{10}\cos \theta = 9$$

Useful Geometric Quantities as Dot Product

Length:

$$|\vec{x}|^2 = \vec{x} \cdot \vec{x} = x_1^2 + x_2^2 + \cdots + x_n^2$$

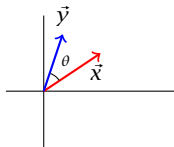
$$|\vec{y}|^2 = \vec{y} \cdot \vec{y}$$

Distance:

$$|\vec{x} - \vec{y}|^2 = \vec{x} \cdot \vec{x} + \vec{y} \cdot \vec{y} - 2\vec{x} \cdot \vec{y}$$

Angle:

$$\cos \theta = \vec{x} \cdot \vec{y} / (|\vec{x}| |\vec{y}|)$$



Dot Product Properties

Some additional properties of the dot product that are useful to know:

$$\vec{x} \cdot \vec{y} = \vec{y} \cdot \vec{x} \text{ (commutative)}$$

$$\vec{x} \cdot (\vec{y} + \vec{z}) = \vec{x} \cdot \vec{y} + \vec{x} \cdot \vec{z} \text{ (distributive)}$$

$$(k\vec{x}) \cdot \vec{y} = \vec{x} \cdot (k\vec{y}) = k(\vec{x} \cdot \vec{y}) \text{ where } k \text{ is a scalar}$$

$$\vec{x} \cdot \vec{y} = 0 \text{ iff } \vec{x} \text{ and } \vec{y} \text{ are orthogonal}$$

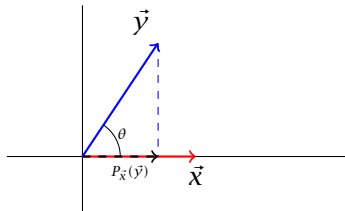
Vector Projection

The projection of \vec{y} onto \vec{x} , $P_{\vec{x}}(\vec{y})$, is the vector obtained by placing \vec{y} and \vec{x} tail to tail and dropping a line, perpendicular to \vec{x} , from the head of \vec{y} onto the line defined by \vec{x} .

$$P_{\vec{x}}(\vec{y}) = \left(\frac{\vec{x} \cdot \vec{y}}{|\vec{x}|} \right) \frac{\vec{x}}{|\vec{x}|} = \left(\frac{\vec{x} \cdot \vec{y}}{|\vec{x}|^2} \right) \vec{x}$$

The component of \vec{y} in \vec{x} , $C_{\vec{x}}(\vec{y})$, is the length of $P_{\vec{x}}(\vec{y})$.

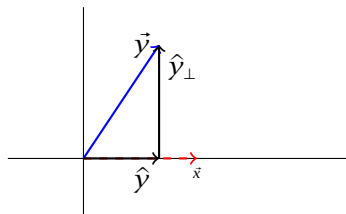
$$C_{\vec{x}}(\vec{y}) = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}|} = |\vec{y}| \cos \theta$$



Vector Projection II

\vec{y} can be decomposed into a vector parallel to \vec{x} , $\hat{y} = P_{\vec{x}}(\vec{y})$, and a vector perpendicular to \vec{x} , \hat{y}_{\perp} .

$$\vec{y} = \hat{y} + \hat{y}_{\perp}$$



- \hat{y}_{\perp} is *orthogonal* to \hat{y} and \vec{x} .
- \hat{y} is the closest vector to \vec{y} in the subspace defined by \vec{x}

Vector Geometry of Simple Statistics

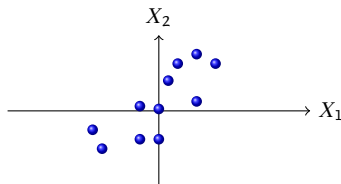
Variable Space Representation of a Data Set

Consider a data set in which we've measured variables

$X = X_1, X_2, \dots, X_p$, on a set of subjects (objects) a_1, \dots, a_n .

	X_1	X_2
a_1	0.9	1.4
a_2	1.1	1.7
\vdots	\vdots	\vdots
a_n	0.5	1.55

Such data is most often represented by drawing the objects as points in space of dimension p . This is the *variable space representation* of the data.



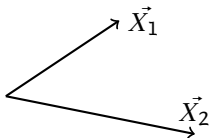
Subject Space Representation of a Data Set

An alternate representation is to consider the variables in the space of the subjects. This is the *subject space* representation.

- trickier to visualize because high dimensional

How then do we come up with a useful representation of variables in subject space?

- Any pair of non-parallel vectors (of arbitrary dimension) defines a plane.
- Let the variables be represented by centered vectors
 - lengths of vectors are proportional to standard deviation
 - angle between vectors represents association or similarity



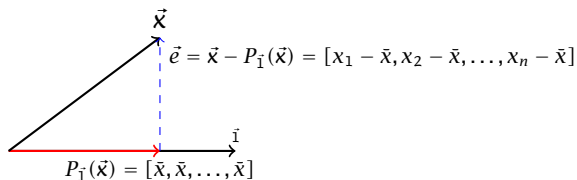
Geometry of the Mean in Subject Space

The mean, as you know, is the ‘optimal’ (in a least square sense) single number summary of a variable of interest.

- The mean, \bar{x} , minimizes the quantity $\sum_{i=1}^n (x_i - \bar{x})^2$.
- The above can be written as $|\vec{x} - \vec{1}\bar{x}|^2$ where $\vec{1} = [1, 1, \dots, 1]'$
- We are looking, therefore, for the scalar multiple, \bar{x} , of the unit vector that minimizes $|\vec{x} - \vec{1}\bar{x}|^2$

Geometry of the Mean in Subject Space II

Geometric derivation of the sample mean:



Geometry of the Mean in Subject Space III

- Recall that:

$$P_{\vec{1}}(\vec{x}) = \vec{1}\bar{x} \text{ for some } \bar{x} \quad (1)$$

$$(\vec{x} - P_{\vec{1}}(\vec{x})) \cdot \vec{1} = 0 \quad (2)$$

- Substituting (1) into (2):

$$(\vec{x} - \vec{1}\bar{x}) \cdot \vec{1} = 0 \quad (3)$$

$$\vec{x} \cdot \vec{1} = \bar{x}(\vec{1} \cdot \vec{1}) \quad (4)$$

- Expanding (4):

$$x_1 + x_2 + \cdots + x_n = n\bar{x} \quad (5)$$

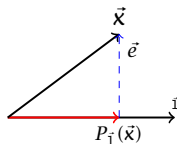
$$\sum x_i = n\bar{x} \quad (6)$$

$$\bar{x} = (1/n) \sum x_i \quad (7)$$

Geometry of Sample Variance

- $|\vec{e}|^2$ is the sum of squared errors (SSE).
- What is the dimensionality of \vec{e} ?
 - Because \vec{e} is orthogonal to the n -dimensional unit vector $\vec{1}$, it must lie in a subspace of dimensionality $n - 1$.
- The mean squared error (MSE) is the average error 'per dimension'

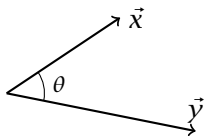
$$\begin{aligned} MSE &= |\vec{e}|^2 / (n - 1) \\ &= \frac{1}{(n - 1)} \sum (x_i - \bar{x})^2 \leftarrow \text{Sample Variance!} \end{aligned}$$



This is a nice geometric demonstration of why the degrees of freedom of the sample variance is $n - 1$.

Correlation in Vector Geometric Terms

Let X and Y be mean centered variables, and let \vec{x} and \vec{y} be their corresponding vector representations in subject space.



$$\text{cor}(X, Y) = r_{XY} = \cos \theta = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}| |\vec{y}|}$$

Bivariate Regression as Projection

The standard bivariate regression equation relating one observed variable X (the predictor) to another observed variable of interest, Y (the outcome) is usually written as:

$$\hat{Y} = a + bX.$$

where \hat{Y} is the predicted value of Y and a and b are scalar values chosen to minimize $|Y - \hat{Y}|$.

Let's express this in vector terms, and work with mean-centered vectors so the equation becomes:

$$\tilde{\hat{y}} = b\tilde{x}$$

See Wickens Chapt 3 for the general derivation for uncentered variables.

Derivation: Bivariate Regression as Projection I

Regression equation for mean-centered vectors: $\hat{\vec{y}} = b\vec{x}$

- Our goal is to choose the scalar b such that the error vector $\vec{e} = \vec{y} - \hat{\vec{y}}$ is as small as possible.
- We've already seen this problem when we derived the mean. We're trying to solve for b in the equation:

$$\begin{aligned}(\vec{y} - b\vec{x}) \cdot \vec{x} &= 0 \\ \vec{x} \cdot \vec{y} &= b(\vec{x} \cdot \vec{x})\end{aligned}$$

- Solving for b we get:

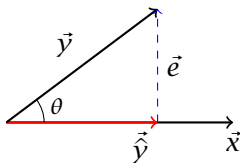
$$b = \frac{\vec{x} \cdot \vec{y}}{(\vec{x} \cdot \vec{x})} = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}|^2}$$

- We can also rewrite $b = (\vec{x} \cdot \vec{y})/|\vec{x}|^2$ as

$$b = \frac{|\vec{x}| |\vec{y}| \cos \theta}{|\vec{x}|^2} = \cos \theta \frac{|\vec{y}|}{|\vec{x}|} = r_{XY} \frac{|\vec{y}|}{|\vec{x}|}$$

Geometry of Bivariate Regression

Geometric interpretation of regression as projection:



$$\hat{\vec{y}} = b\vec{x}$$

$$\begin{aligned} b &= |\vec{x}||\vec{y}| \cos \theta / |\vec{x}|^2 \\ &= \cos \theta (|\vec{y}| / |\vec{x}|) \\ &= r_{XY} (|\vec{y}| / |\vec{x}|) \end{aligned}$$

Bivariate Regression, Goodness of Fit

How well does our prediction agree with our outcome?

- Measure the angle between $\vec{\hat{y}}$ and \vec{y} :

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

- In the single-predictor case $R = r_{XY}$, but this is not generally true when we have multiple predictors.
- Note that $|\vec{y}|$ can be expressed as follows:

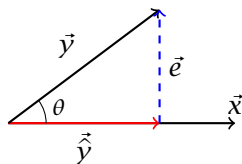
$$\begin{aligned} |\vec{\hat{y}}|^2 + |\vec{e}|^2 &= |\vec{y}|^2 \\ SS_{\text{regression}} + SS_{\text{residual}} &= SS_{\text{total}} \end{aligned}$$

- With simple substitution we can show that:

$$\begin{aligned} SS_{\text{regression}} &= R^2 SS_{\text{total}} \\ SS_{\text{residual}} &= (1 - R^2) SS_{\text{total}} \end{aligned}$$

Geometry of Goodness of Fit

Geometric interpretation of regression goodness-of-fit:



$$R = \cos \theta$$

$$|\vec{\hat{y}}|^2 + |\vec{e}|^2 = |\vec{y}|^2$$