Scientific Computing for Biologists

Data as Vectors: Geometry of Bivariate Relationships

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Overview of Lecture

- Variable space/Subject space representations
- 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
  - Mean as projection in subject space
  - Bivariate regression in geometric terms
  - Difference in group means as a regression problem

Hands-on Session

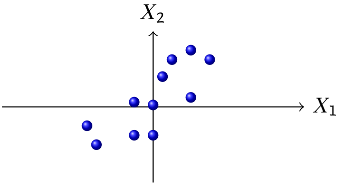
- Visualizing bivariate relationships in R
- Vector mathematics in R
- Writing functions in R
- Correlation and linear regression in R

Variable Space Representation of a Data Set

Consider a data set in which we've measured variables
$\mathsf{X} = X_1, X_2, \ldots, X_p$, on a set of subjects (objects) $a_1, ..., a_n$.

	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.

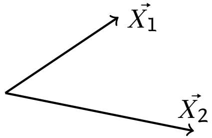


Subject Space Representation of a Data Set

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

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

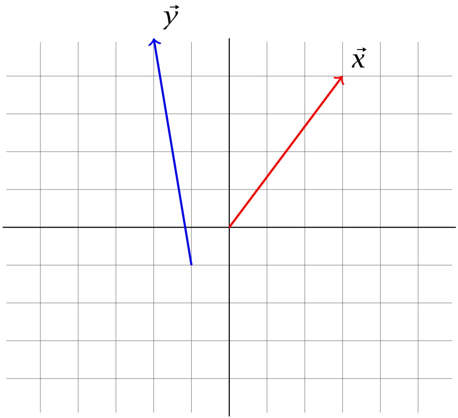
- Let the variables be represented by centered vectors
  - lengths of vectors are proportional to standard deviation
  - angle between vectors represents association or similarity



This representation of variables as vectors in the space of the subjects is the view that we'll develop over the next few lectures.

Vector Geometry

Vectors are directed line segments.

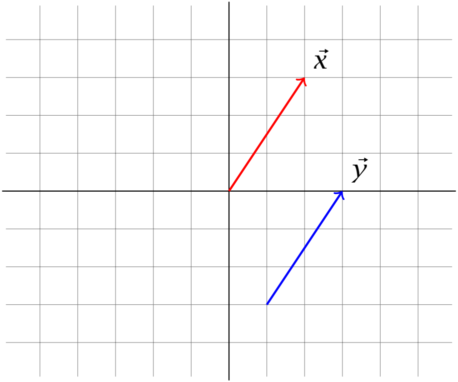


All of the figures and algebraic formulas I show you apply to n-dimensional vectors.

Vector Geometry

Vectors have direction and length:

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

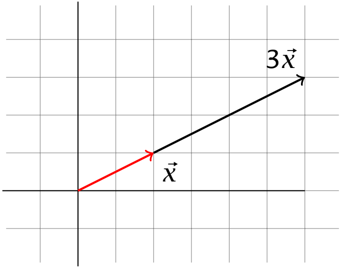


Often starting point is ignored, in which case $\vec{x} = \vec{y}$.

Scalar Multiplication of a Vector

Let k be a scalar.

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

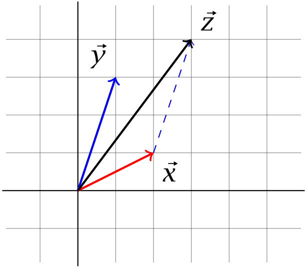


$\vec{x} = [2, 1]'$; $3\vec{x} = [6, 3]'$.

Vector Addition

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

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

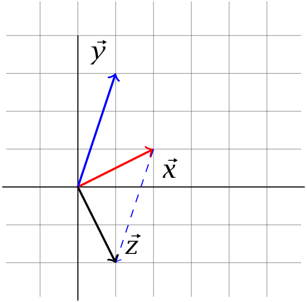


Addition follows the ‘head-to-tail’ rule.

Vector Subtraction

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

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

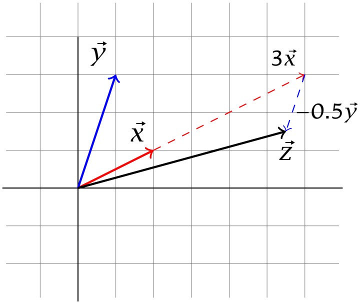


Follow the addition rule for $-1\vec{y}$.

Linear Combinations of Vectors

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

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

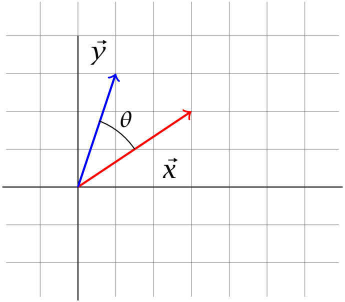


Dot Product

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

$$\begin{aligned}\vec{x} \cdot \vec{y} &= x_1 y_1 + x_2 y_2 + \cdots + x_n y_n \\ &= |\vec{x}||\vec{y}| \cos\theta\end{aligned}$$

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:

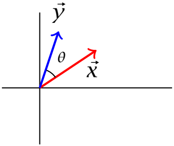
$$
\begin{aligned}
|\vec{x}|^2 &= \vec{x} \cdot \vec{x} = x_1^2 + x_2^2 + \cdots + x_n^2 \\
|\vec{y}|^2 &= \vec{y} \cdot \vec{y}
\end{aligned}
$$

Distance:

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

Angle:

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



Dot Product Properties

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

$$
\begin{aligned}
\vec{x} \cdot \vec{y} &= \vec{y} \cdot \vec{x} \text{ (commutative)} \\
\vec{x} \cdot (\vec{y} + \vec{z}) &= \vec{x} \cdot \vec{y} + \vec{x} \cdot \vec{z} \text{ (distributive)} \\
(k\vec{x}) \cdot \vec{y} &= \vec{x} \cdot (k\vec{y}) = k(\vec{x} \cdot \vec{y}) \text{ where } k \text{ is a scalar} \\
\vec{x} \cdot \vec{y} &= 0 \text{ iff } \vec{x} \text{ and } \vec{y} \text{ are orthogonal}
\end{aligned}
$$

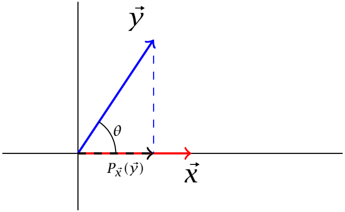
Vector Projection

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 $P_{\vec{x}}(\vec{y})$.

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

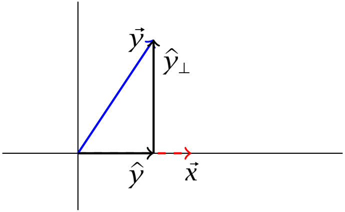


Vector Projection II

$\vec{y}$ can be decomposed into two parts:

1. a vector parallel to $\vec{x}$, $\hat{y} = P_{\vec{x}}(\vec{y})$,
2. a vector perpendicular to $\vec{x}$, $\hat{y}_\perp$.

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

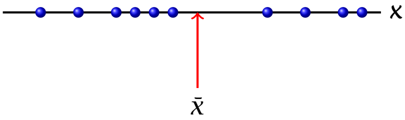


- $\hat{y}_\perp$ is *orthogonal* to $\hat{y}$ and $\vec{x}$.
- $\hat{y}$ is the closest vector to $\vec{y}$ in the subspace defined by $\vec{x}$

Vector Geometry of Simple Statistics

Geometry of the Mean in Variables Space

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

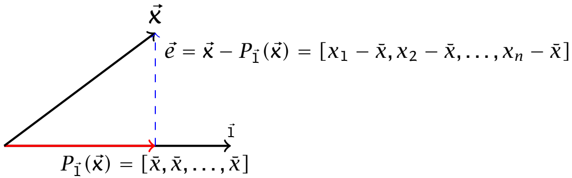


The mean, $\bar{x}$, minimizes the quantity:

$$\sum_{i=1}^{n} (x_i - \bar{x})^2$$

Geometry of the Mean in Subject Space

- 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 $\vec{1} = [1, 1, \ldots, 1]'$
- We are looking, therefore, for the scalar multiple, $\bar{x}$, of the unit vector that minimizes $|\vec{x} - \vec{1}\bar{x}|^2 = |\vec{e}|$



Geometry of the Mean in Subject Space II

- Recall that:

$$
\begin{aligned}
P_{\vec{1}}(\vec{x}) &= \vec{1}\bar{x} \text{ for some } \bar{x} && (1)\\
(\vec{x} - P_{\vec{1}}(\vec{x})) \cdot \vec{1} &= 0 && (2)
\end{aligned}
$$

- Substituting (1) into (2):

$$
\begin{aligned}
(\vec{x} - \vec{1}\bar{x}) \cdot \vec{1} &= 0 && (3)\\
\vec{x} \cdot \vec{1} &= \bar{x}(\vec{1} \cdot \vec{1}) && (4)
\end{aligned}
$$

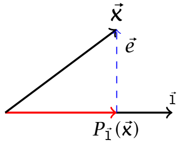
- Expanding (4):

$$
\begin{aligned}
x_1 + x_2 + \cdots + x_n &= n\bar{x} && (5)\\
\sum x_i &= n\bar{x} && (6)\\
\bar{x} &= (1/n) \sum x_i && (7)
\end{aligned}
$$

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 subpace of dimensionality $n-1$.
- The mean squared error (MSE) is the average error 'per dimension'

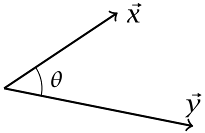
$$\begin{aligned} MSE &= |\vec{e}|^2/(n-1) \\ &= \frac{1}{(n-1)} \sum (x_i - \bar{x})^2 \leftarrow \textbf{Sample Variance!} \end{aligned}$$



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.



We can write the correlation in vectors terms:

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

Compare to conventional algebraic formula:

$$r_{XY} = \frac{E[(X - \bar{x})(Y - \bar{y})]}{\sigma_x \sigma_y}$$

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 $|Y - \hat{Y}|$.

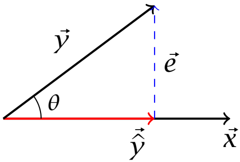
Let's express this in vector terms, and work with mean-centered vectors so the equation becomes:

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

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

Geometry of Bivariate Regression

Geometric interpretation of regression as projection:



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

$$b \quad = \quad ?$$

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:

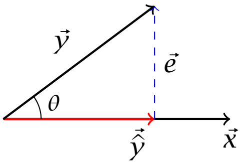
$$
b = \frac{\vec{x} \cdot \vec{y}}{(\vec{x} \cdot \vec{x})} = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}|^2}
$$

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

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

Geometry of Bivariate Regression

Geometric interpretation of regression as projection:



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

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

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:

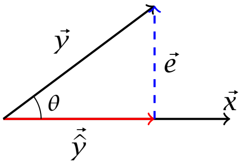
$$\begin{aligned} |\vec{\hat{y}}|^2 + |\vec{e}|^2 &= |\vec{y}|^2 \\ SS_{regression} + SS_{residual} &= SS_{total} \end{aligned}$$

- With simple substitution we can show that:

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

Geometry of Goodness of Fit

Geometric interpretation of regression goodness-of-fit:



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

The better the goodness-of-fit, the smaller the angle, $\cos\theta$, and the shorter residual vector, $\vec{e}$.

Two-group ANOVA as Regression

We can also use a geometric perspective to test whether the mean of a variable differs between two groups of subjects.

- Setup a 'dummy variable' as the predictor X_g. We assign all subjects in group 1 the value 1 and all subjects in group 2 the value -1 on the dummy variable. We then regress the variable of interest, Y, on X_g.
- When the means are different in the two groups, X_g will be a good predictor of the variable of interest, hence $\vec{y}$ and $\vec{x_g}$ will have a small angle between them.
- When the means in the two groups are similar, the dummy variable will not be a good predictor. Hence the angle between $\vec{y}$ and $\vec{x_g}$ will be large.