Scientific Computing for Biologists

Data as Vectors

Instructor: Paul M. Magwene

06 September 2011

Overview of Lecture

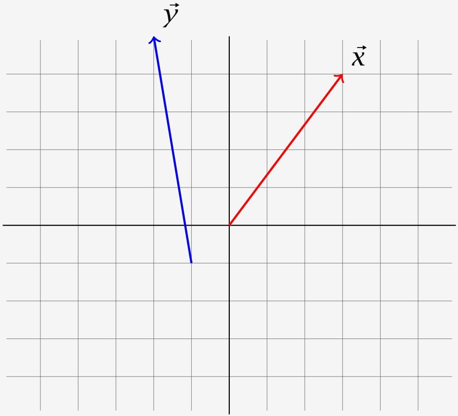
- Vector Geometry
  - Vectors are directed line segments
  - Vector length
- Vector Arithmetic
  - Addition, subtraction
  - Scalar multiplication
  - Linear combinations of vectors
  - Dot product and projection
- Vector representations of multivariate data
  - Variable space/Subject space representations
  - 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 and Python
- Writing functions in R and Python
- Visualizing univariate distributions on R
- Linear regression and t-tests in R

Vector Geometry

Vectors are directed line segments.

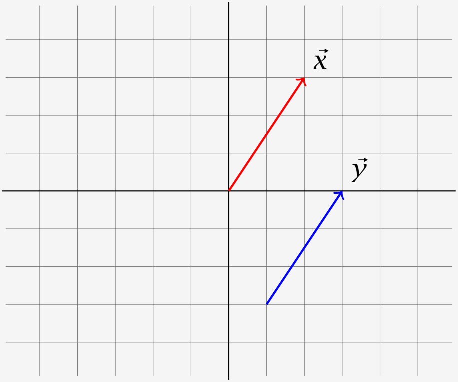


All of the figures and algebraic formulas I show you apply to n-dimensional vectors.

Vector Geometry

Vectors have direction and length:

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

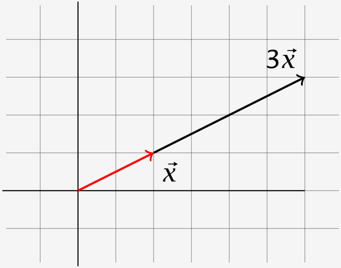


Often starting point is ignored, in which case $\vec{x} = \vec{y}$.

Scalar Multiplication of a Vector

Let k be a scalar.

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

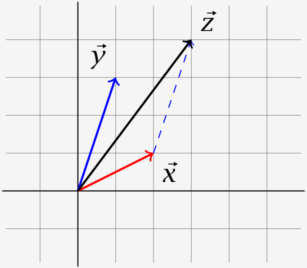


$\vec{x} = [2, 1]'$; $3\vec{x} = [6, 3]'$.

Vector Addition

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

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

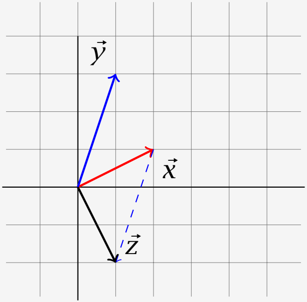


Addition follows the ‘head-to-tail’ rule.

Vector Subtraction

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

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

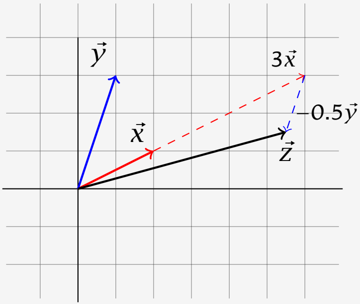


Follow the addition rule for $-1\vec{y}$.

Linear Combinations of Vectors

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

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

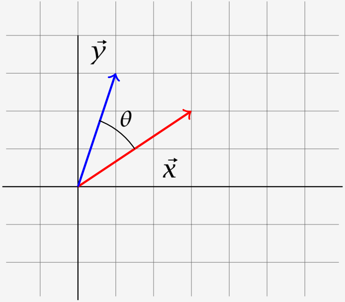


Dot Product

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:

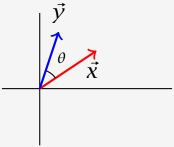
$$
\begin{aligned}
|\vec{x}|^2 &= \vec{x} \cdot \vec{x} = x_1^2 + x_2^2 + \cdots + x_n^2 \\
|\vec{y}|^2 &= \vec{y} \cdot \vec{y}
\end{aligned}
$$

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:

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

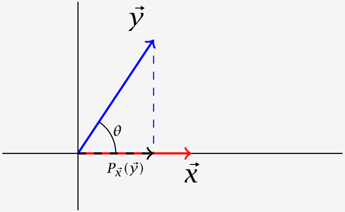
Vector Projection

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

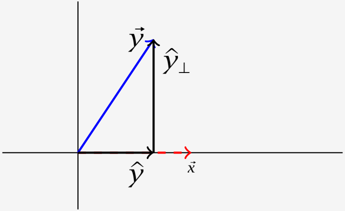
$$C_{\vec{x}}(\vec{y}) = \frac{\vec{x}\cdot\vec{y}}{|\vec{x}|} = |\vec{y}|\cos\theta$$



Vector Projection II

$\vec{y}$ can be decomposed into a 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 $\vec{x}$

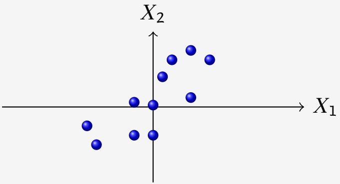
Vector Geometry of Simple Statistics

Variable Space Representation of a Data Set

Consider a data set in which we've measured variables $\mathsf{X} = X_1, X_2, \ldots, X_p$, 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.



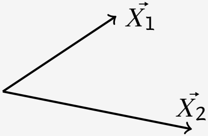
Subject Space Representation of a Data Set

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

- 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



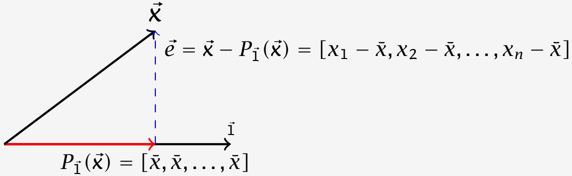
Geometry of the Mean in Subject Space

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

Geometry of the Mean in Subject Space II

Geometric derivation of the sample mean:



Geometry of the Mean in Subject Space III

- 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):

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

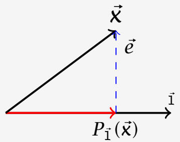
- Expanding (4):

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

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'

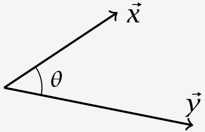
$$\begin{aligned} MSE &= |\vec{e}|^2/(n-1) \\ &= \frac{1}{(n-1)} \sum (x_i - \bar{x})^2 \leftarrow \textbf{Sample Variance!} \end{aligned}$$



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.



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

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:

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

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

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.

Derivation: Bivariate Regression as Projection I

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

- Our goal is to choose the scalar b such that the error vector $\vec{e} = \vec{y} - \vec{\hat{y}}$ 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:

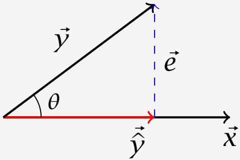
$$b = \frac{\vec{x} \cdot \vec{y}}{(\vec{x} \cdot \vec{x})} = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}|^2}$$

- 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:



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

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

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:

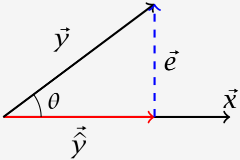
$$\begin{aligned} |\vec{\hat{y}}|^2 + |\vec{e}|^2 &= |\vec{y}|^2 \\ SS_{regression} + SS_{residual} &= SS_{total} \end{aligned}$$

- 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:



$$R = \cos\theta$$

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

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.