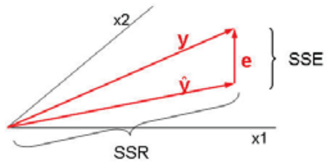
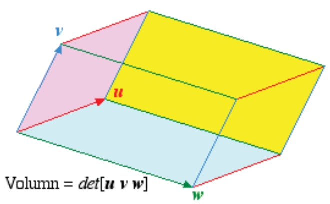


$$\begin{bmatrix} 3 & 2 \\ 1 & -3 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \end{pmatrix}$$

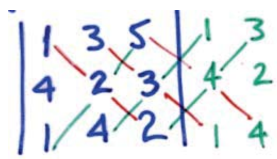
$$\underset{2\times 2}{A} \; \underset{2\times 1}{\underset{\sim}{x}} = \underset{2\times 1}{b}$$

$$\mathbf{R}\begin{pmatrix} \mathbf{x} \\ \hline \mathbf{y} \end{pmatrix} = \left[\begin{array}{c|c} \mathbf{R}_{XX} & \mathbf{R}_{XY} \\ \hline \mathbf{R}_{YX} & \mathbf{R}_{YY} \end{array}\right]$$

Vectors & Matrices
with statistical applications



Michael Friendly
Psychology 6140



Why learn matrix algebra?

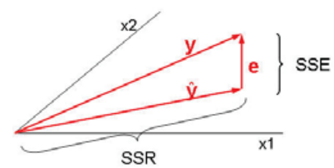
- Simple way to express linear combinations of variables and general solutions of equations.

$$\begin{cases} \mathbf{a}'\mathbf{x} = a_1x_1 + a_2x_2 + a_3x_3 \\ \mathbf{A}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{b}_{n\times 1} \Rightarrow \mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \end{cases}$$

- Linear statistical models (regression, anova) generalize to any # of predictors & responses.

$$\begin{cases} \hat{y}_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \\ \hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\beta} \quad \text{univariate response} \\ \hat{\mathbf{Y}} = \mathbf{XB} \quad \text{multivariate response} \end{cases}$$

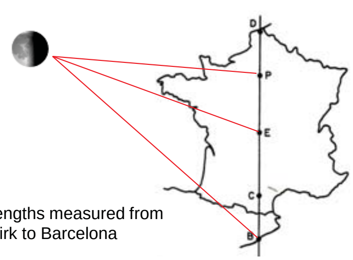
- Strong relations between algebra, geometry & statistical concepts



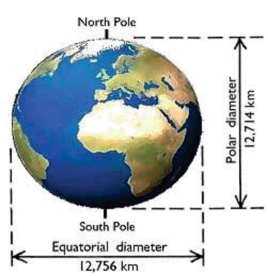
Goal: a *reading* knowledge of matrix expressions to aid in understanding statistical concepts.

Brief history of linear algebra

- Ideas first arose in relation to solving systems of equations in astronomy & geodesy (1700s)
  - Determining the "shape of the earth" from measures of latitude and arc length (3 eqn., 3 unknowns)
  - Calculating the orbits of planets, e.g., Saturn, Jupiter (6 eqn., 6 unknowns)



Arc lengths measured from Dunkirk to Barcelona

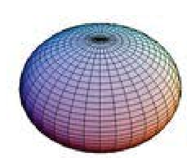


Pierre-Louis Moreau de Maupertius

"*The man who flattened the earth*"

(Portrait from 1739)

His crowning glory was a journey to Lapland, making measures of the length of 1º of latitude, and showing that they were smaller near the poles than at the equator.



Brief history of linear algebra

- By ~ 1800, Gauss developed "Gaussian elimination" to solve such problems, and "least squares" to deal with fallible measurements
- Still required proper notation & algebra (**A** $_{m \times n}$)
  - 1848: J.J. Sylvester introduced "matrix" (Latin: womb) for array of numbers, with a *single symbol*.
  - 1855: Arthur Cayley defined matrix multiplication in relation to systems of equations
  - 1858: Cayley develops algebra, including inverse, $\mathbf{A}^{-1}$
- Now, there was a **general** notation for solving m equations in n unknowns!

Vectors & matrices

- A *matrix* is a rectangular array of numbers, with r rows and c columns.

$$\mathbf{A}_{3\times 2} = \begin{bmatrix} 12 & 3 \\ 15 & 0 \\ 7 & -1 \end{bmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix} = (a_{ij}), \ {}_{\substack{i=1,2,\dots r \\ j=1,2,\dots c}}$$

$$\mathbf{B}_{2\times 3} = \begin{pmatrix} 1 & 7 & -3 \\ 2 & 4 & 6 \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{pmatrix}$$

Transpose operation: $\mathbf{A}' \equiv \mathbf{A}^T = [a_{ji}]$, interchanges rows and columns

$$\mathbf{B}'_{3\times 2} = \begin{pmatrix} 1 & 2 \\ 7 & 4 \\ -3 & 6 \end{pmatrix}$$

Vectors & matrices

- A *vector* is just a one column matrix
- Sometimes written in transposed (row) form to save space.

$$\mathbf{y}_{3\times 1} = \begin{pmatrix} 6 \\ 7 \\ 12 \end{pmatrix}$$

$$\mathbf{y}'_{1\times 3} \equiv \mathbf{y}^T{}_{1\times 3} = \begin{pmatrix} 6 & 7 & 12 \end{pmatrix}$$

$$\mathbf{y}_{3\times 1} = \begin{pmatrix} 6 & 7 & 12 \end{pmatrix}'$$

All of these forms define **y** as a 3 x 1 column vector

Special vectors & matrices

unit vector: $\underset{\sim}{\mathbf{1}}_n \equiv \underset{\sim}{\mathbf{j}}_n = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}_n$

zero vector: $\underset{\sim}{\mathbf{0}}_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_n$

contrast vectors: $\sum^n c_i = 0$

$$\mathbf{c}'_1 = \begin{pmatrix} 1 & 1 & -1 & -1 \end{pmatrix}$$

$$\mathbf{c}'_2 = \begin{pmatrix} 3 & -1 & -1 & -1 \end{pmatrix}$$

Square matrix: $\mathbf{A}_{n \times n}$: same # rows/cols

$$\mathbf{A}_{2\times 2} = \begin{bmatrix} 2 & 10 \\ 11 & 9 \end{bmatrix} \qquad \mathbf{B}_{3\times 3} = \begin{bmatrix} 9 & 7 & 1 \\ 3 & 3 & 5 \\ 1 & 9 & 4 \end{bmatrix}$$

Symmetric matrix: $\mathbf{A} = \mathbf{A}^T$, or $a_{ij}=a_{ji}$

$$\mathbf{A}_{2\times 2} = \begin{bmatrix} 2 & 10 \\ 10 & 9 \end{bmatrix} \qquad \mathbf{B}_{3\times 3} = \begin{bmatrix} 9 & 7 & 1 \\ 7 & 3 & 5 \\ 1 & 5 & 4 \end{bmatrix}$$

Diagonal matrix: $a_{ij} = 0$ for $i \neq j$

$$\mathbf{D}_{2\times 2} = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} \qquad \mathbf{D}_{3\times 3} = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 6 \end{bmatrix}$$

Special vectors & matrices

Identity matrix: diagonal w/ $a_{ii} = 1$

$$\mathbf{I}_{2\times2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \mathbf{I}_{3\times3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Why: acts like 1 in multiplication–

A I = A

Unit matrix: all $a_{ij} = 1$

$$\mathbf{J}_{3\times2} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{j}_3 & \mathbf{j}_3 \end{bmatrix}$$

Why: convenient way to sum vectors & matrices

$\mathbf{a}^\mathsf{T}\mathbf{j} = \sum a_i$

Zero matrix: all $a_{ij} = 0$

$$\mathbf{0}_{2\times3} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Why: acts like 0 in addition—

A + 0 = A

A - B = 0 $\rightarrow$ **A = B**

Operations on vectors & matrices

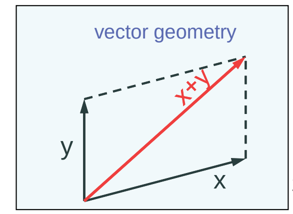
Addition & subtraction: add corresponding elements. Must have same shape

$$\mathbf{a}_{3\times1} + \mathbf{b}_{3\times1} = (a_i + b_i) = \begin{pmatrix} a_1 + b_1 \\ a_2 + b_2 \\ a_3 + b_3 \end{pmatrix} \qquad \mathbf{A}_{3\times2} + \mathbf{B}_{3\times2} = \begin{bmatrix} a_{ij} + b_{ij} \end{bmatrix} = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} \\ a_{21} + b_{21} & a_{22} + b_{22} \\ a_{31} + b_{31} & a_{32} + b_{32} \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 10 & 2 \\ 4 & 6 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 5 & 3 \\ 4 & 4 \end{bmatrix} \Rightarrow \mathbf{A} + \mathbf{B} = \begin{bmatrix} 15 & 5 \\ 8 & 10 \end{bmatrix} \quad \mathbf{A} - \mathbf{B} = \begin{bmatrix} 5 & -1 \\ 0 & 2 \end{bmatrix}$$

Properties: same as for scalars– order doesn't matter

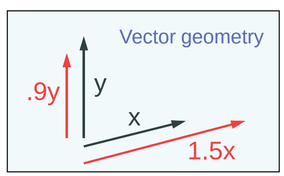
- Commutative: **A** + **B** = **B** + **A**
- Associative: **A** + (**B** + **C**) = (**A** + **B**) + **C**



Operations on vectors & matrices

Scalar multiplication: multiply each element by a scalar.

$$k\mathbf{a}_{n\times1} = (ka_i) = \begin{pmatrix} ka_1 \\ \vdots \\ ka_n \end{pmatrix} \qquad c\mathbf{A}_{m\times n} = \begin{bmatrix} ca_{ij} \end{bmatrix} = \begin{pmatrix} ca_{11} & \cdots & ca_{1n} \\ \vdots & \ddots & \vdots \\ ca_{m1} & \cdots & ca_{mn} \end{pmatrix}$$



$$3\begin{pmatrix} 1 \\ 5 \\ 10 \end{pmatrix} = \begin{pmatrix} 3 \\ 15 \\ 30 \end{pmatrix} \qquad 2\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 2 & 4 \\ 6 & 8 \end{bmatrix} \qquad \lambda\mathbf{I}_{n\times n} = \begin{bmatrix} \lambda & 0 & \cdots & 0 \\ 0 & \lambda & \cdots & 0 \\ 0 & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \lambda \end{bmatrix}$$

$$R - \lambda\mathbf{I} = \begin{bmatrix} 1-\lambda & r_{12} & r_{13} \\ r_{21} & 1-\lambda & r_{23} \\ r_{31} & r_{32} & 1-\lambda \end{bmatrix}$$

Partitioned matrices

Def^n : A partitioned matrix has its rows & columns divided into sub-matrices

$$\mathbf{A}_{4\times3} = \left[\begin{array}{cc|c} 1 & 2 & 3 \\ 4 & 5 & 6 \\ \hline 7 & 8 & 9 \\ 10 & 11 & 12 \end{array}\right] = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$$

Same matrix, just with names for the sub-matrices

$$\mathbf{A}_{21} = \begin{bmatrix} 7 & 8 \\ 10 & 11 \end{bmatrix}$$

Makes it easier to express sets of variables

Statistical examples:

$$\mathbf{R}\left(\begin{array}{c} \mathbf{x} \\ \hline \mathbf{y} \end{array}\right) = \left[\begin{array}{c|c} \mathbf{R}_{XX} & \mathbf{R}_{XY} \\ \hline \mathbf{R}_{YX} & \mathbf{R}_{YY} \end{array}\right] \qquad (\mathbf{X} \mid \mathbf{y})'(\mathbf{X} \mid \mathbf{y}) = \left[\begin{array}{c|c} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{y} \\ \hline \mathbf{y}'\mathbf{X} & \mathbf{y}'\mathbf{y} \end{array}\right]$$

Partitioned matrices

Addition and subtraction is defined for partitioned matrices if all submatrices in corresponding positions are of the same size and shape

$$\left[\begin{array}{cc:c} 1 & 2 & 3 \\ 4 & 5 & 6 \\ \hdashline 7 & 8 & 9 \end{array}\right] + \left[\begin{array}{cc:c} 2 & 2 & 0 \\ 1 & 0 & -1 \\ \hdashline 0 & 2 & -1 \end{array}\right] = \left[\begin{array}{cc:c} 3 & 4 & 3 \\ 5 & 5 & 5 \\ \hdashline 7 & 10 & 8 \end{array}\right]$$

Symbolically,

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} + \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{11}+\mathbf{B}_{11} & \mathbf{A}_{12}+\mathbf{B}_{12} \\ \mathbf{A}_{21}+\mathbf{B}_{21} & \mathbf{A}_{22}+\mathbf{B}_{22} \end{bmatrix}$$

Vector & matrix multiplication

Vector x vector
(inner product)

$$\underset{1\times n}{\underline{a}'}\ \underset{n\times 1}{\underline{x}} = (a_1\ a_2 \cdots a_n)\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

$$= a_1x_1 + a_2x_2 + \cdots + a_nx_n$$

$$= \sum_{i=1}^{n} a_i x_i$$

sum of products of corresponding elements

eg: $(1\ \ -2\ \ 1)\begin{pmatrix} 12 \\ 20 \\ 40 \end{pmatrix} = 1\cdot 12 + (-2)\cdot 20 + 1\cdot 40 = 12$

NB: $\underline{a}'\underline{x} \equiv \underline{x}'\underline{a}$

Note that inner dimensions must match!

Vector & matrix multiplication

special cases

(a) $\underline{y}'\underline{y} = (y_1, \cdots, y_n)\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} = y_1^2 + y_2^2 + \cdots y_n^2 = \sum_{i=1}^{n} y_i^2$

(b) $\underline{1}'\underline{y} = (1\ 1 \cdots 1)\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = y_1 + y_2 + \cdots y_n = \sum y_i$

$= \underline{y}'\underline{1}$

(c) $\left.\begin{array}{l} \underline{a}'\underline{0} = 0 \\ \underline{0}'\underline{a} = 0 \end{array}\right\}$ $(1\ \ 3\ \ 5)\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = 0$

Geometry of vector products

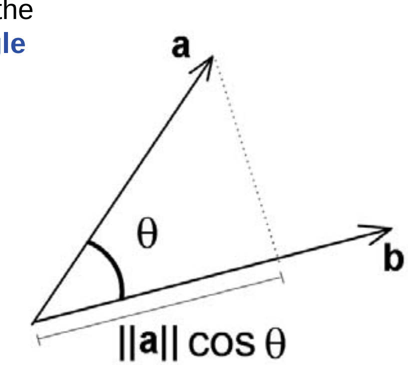
- In a geometric representation, the scalar product relates to the **angle** between 2 vectors:

$$\mathbf{a}'\mathbf{b} = \|\mathbf{a}\| \cdot \|\mathbf{b}\| \cdot \cos\theta$$

- **Orthogonal** vectors (θ=90) have the property that **a′ b** = 0

$$\mathbf{a}'\mathbf{b} = (1\ \ 1\ \ 1)\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} = 0$$

- **Correlation** (= cos θ) = $\dfrac{\mathbf{x}'\mathbf{y}}{\|\mathbf{x}\| \cdot \|\mathbf{y}\|}$



Matrix product

The matrix product, **A B**, is defined only if

the # of columns of A = # of rows of B

Then, **A** and **B** are conformable for multiplication

$$\begin{bmatrix}1&2&3\\4&5&6\end{bmatrix}\begin{bmatrix}1&1&1\\2&2&2\\3&3&3\end{bmatrix}$$

(2×3) ✓ (3×3)

$$\begin{bmatrix}1&1&1\\2&2&2\\3&3&3\end{bmatrix}\begin{bmatrix}1&2&3\\4&5&6\end{bmatrix}$$

(3×3) (2×3) Not conformable

Matrix product

Algebraic view:

matrix x matrix

Let $\underset{r\times c}{A} = [a_{ik}]$ $\quad i=1,\cdots r$, $k=1,\cdots c$

$\underset{c\times s}{B} = [b_{kj}]$ $\quad k=1,\cdots c$, $j=1,\cdots s$

Then

$$\underbrace{\underset{r\times c}{A}\cdot\underset{c\times s}{B}}_{\text{product}} = \underset{r\times s}{C} = [c_{ij}] = [\underline{a}_i'\,\underline{b}_j]$$

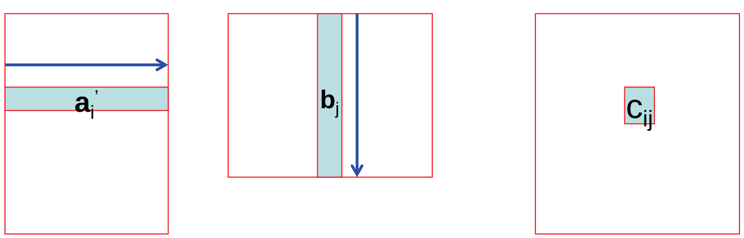
rows of A • cols of B

Each element, c_{ij} is the vector product of row *i* of A times col *j* of B

Matrix product

$\mathbf{A}_{rc}$ * $\mathbf{B}_{cs}$ = $\mathbf{C}_{rs}$

Diagram view



Vector formula $\quad \boldsymbol{a}_i' \quad \boldsymbol{b}_j \quad = \quad c_{ij}$

Scalar formula

$$\begin{pmatrix}a_{i1} & a_{i2} & \cdots & a_{ic}\end{pmatrix}\begin{pmatrix}b_{1j}\\ b_{2j}\\ \vdots \\ b_{cj}\end{pmatrix} = \sum_{k=1}^{c} a_{ik}b_{kj} = c_{ij}$$

Matrix product: examples

e.g. A B

$$\begin{pmatrix}1&1&2\\4&0&-1\end{pmatrix}\begin{pmatrix}2&0\\1&1\\0&3\end{pmatrix} = \begin{pmatrix}2+1+0 & 0+1+6\\ 8+0+0 & 0+0-3\end{pmatrix} = \begin{pmatrix}3&7\\8&-3\end{pmatrix}$$

2×3 ✓ 3×2 $\qquad 2\times 2$

A B

$$\begin{pmatrix}1&2\\3&4\end{pmatrix}\begin{pmatrix}0&3\\2&1\end{pmatrix} = \begin{pmatrix}4&5\\8&13\end{pmatrix}$$

NB $AB \neq BA$

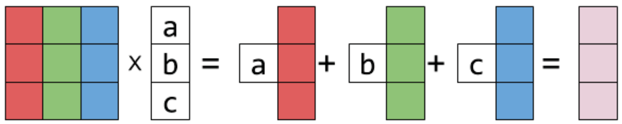
$$\begin{pmatrix}0&3\\2&1\end{pmatrix}\begin{pmatrix}1&2\\3&4\end{pmatrix} = \begin{pmatrix}9&12\\5&8\end{pmatrix}$$

B A

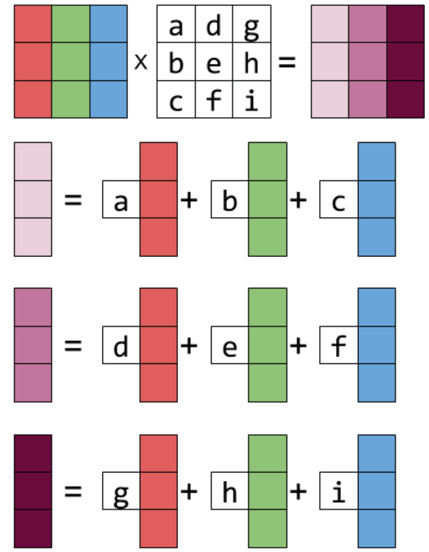
Visualizing matrix product

- Right-mult: linear combination of columns

multiplying A by B is the linear combination of the columns of A
using coefficients from B



$$\begin{pmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{pmatrix} * \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} ax_1 + by_1 + cz_1 \\ ax_2 + by_2 + cz_2 \\ ax_3 + by_3 + cz_3 \end{pmatrix}$$



Right multiplying by a matrix is just more of the same.

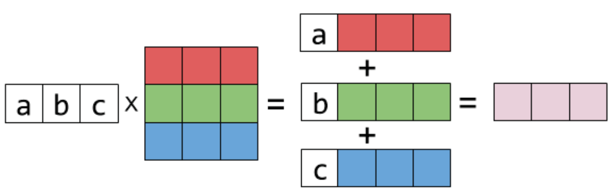
Each column of the result is a different linear combination of the columns of A

$$\begin{pmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{pmatrix} * \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & i \end{pmatrix} = \begin{pmatrix} ax_1 + by_1 + cz_1 & dx_1 + ey_1 + fz_1 & gx_1 + hy_1 + iz_1 \\ ax_2 + by_2 + cz_2 & dx_2 + ey_2 + fz_2 & gx_2 + hy_2 + iz_2 \\ ax_3 + by_3 + cz_3 & dx_3 + ey_3 + fz_3 & gx_3 + hy_3 + iz_3 \end{pmatrix}$$

Visualizing matrix product

- Left-mult: linear combination of rows

multiplying A by B is the linear combination of the rows of B
using coefficients from A



$$\begin{pmatrix} a & b & c \end{pmatrix} * \begin{pmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{pmatrix} = \begin{pmatrix} ax_1 + bx_2 + cx_3 & ay_1 + by_2 + cy_3 & az_1 + bz_2 + cz_3 \end{pmatrix}$$

From: http://eli.thegreenplace.net/2015/visualizing-matrix-multiplication-as-a-linear-combination

Why multiply like this?

To express systems of linear equations:

$$\begin{matrix} 3x_1 + 2x_2 = 4 \\ x_1 - 3x_2 = 0 \end{matrix} \iff \begin{bmatrix} 3 & 2 \\ 1 & -3 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \end{pmatrix}$$

$$\underset{2\times2}{A} \quad \underset{2\times1}{\underline{x}} = \underset{2\times1}{\underline{b}}$$

In general:

$$\left.\begin{matrix} m \text{ equations} \\ n \text{ unknowns} \end{matrix}\right\} \rightarrow \underset{(m\times n)}{A} \quad \underset{(n\times1)}{\underline{x}} = \underset{(m\times1)}{b}$$

Solution: $\mathbf{x} = \mathbf{A}^{-1}\,\mathbf{b}$ when $\mathbf{A}^{-1}$ exists (m=n, eqn. independent)

Properties of matrix multiplication

1. Associative $\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C}$
2. Distributive $(\mathbf{A}+\mathbf{B})\mathbf{C} = \mathbf{AC}+\mathbf{BC}$
   $\mathbf{A}(\mathbf{B}+\mathbf{C}) = \mathbf{AB}+\mathbf{AC}$
3. NOT commutative (in general) $\mathbf{AB} \neq \mathbf{BA}$
4. Identity $\underset{r\times c}{\mathbf{A}}\ \underset{c\times c}{\mathbf{I}} = \underset{r\times r}{\mathbf{I}}\ \underset{r\times c}{\mathbf{A}} = \mathbf{A}$

$$\begin{pmatrix}1 & 2 & 3\\ 4 & 5 & 6\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix}1 & 2 & 3\\ 4 & 5 & 6\end{pmatrix}$$

Properties of matrix multiplication

5. Zero $\mathbf{A}_{r\times c}\ \mathbf{0}_{c\times s} = \mathbf{0}_{r\times s}$
6. Transpose of a product $(\mathbf{AB})^T = \mathbf{B}^T\ \mathbf{A}^T$
   $(\mathbf{AB}\cdots\mathbf{Z})^T = \mathbf{Z}^T \cdots \mathbf{B}^T\ \mathbf{A}^T$

All of these properties are analogous to ordinary (scalar) algebra, except for (3) and (6). Why?

Matrix powers

For a **square** matrix, A $_{(n \times n)}$:

$$\mathbf{A}^2 = \mathbf{A}\ \mathbf{A}$$

$$\mathbf{A}^3 = \mathbf{A}\ \mathbf{A}\ \mathbf{A} = \mathbf{A}^2\mathbf{A}$$ etc, for A^p

e.g., $$\begin{pmatrix}1 & 2\\ 3 & 4\end{pmatrix}^2 = \begin{pmatrix}1 & 2\\ 3 & 4\end{pmatrix}\begin{pmatrix}1 & 2\\ 3 & 4\end{pmatrix} = \begin{pmatrix}7 & 10\\ 15 & 22\end{pmatrix}$$

In applications (e.g., MAP II-1), matrix powers provide a simple way to compute paths through a network, represented by (0/1) values in a matrix.

Matrix powers

Square roots too:

If $\mathbf{B}^2 = \mathbf{A}$, then $\mathbf{B}$ is also the square root of $\mathbf{A}$, i.e., $\mathbf{B} = \mathbf{A}^{1/2}$

e.g., $$\begin{pmatrix}4 & 0\\ 0 & 3\end{pmatrix}^2 = \begin{pmatrix}4 & 0\\ 0 & 3\end{pmatrix}\begin{pmatrix}4 & 0\\ 0 & 3\end{pmatrix} = \begin{pmatrix}16 & 0\\ 0 & 9\end{pmatrix} = \mathbf{A}$$

so, $$\begin{pmatrix}16 & 0\\ 0 & 9\end{pmatrix}^{1/2} = \begin{pmatrix}4 & 0\\ 0 & 3\end{pmatrix} = \mathbf{B} = \mathbf{A}^{1/2}$$

The idea of the "square root of a matrix" was fundamental in the development of factor analysis, where Thurstone defined factors as

$$\boxed{\mathbf{R}} \approx \boxed{\Lambda}\ \boxed{\Lambda'}$$

Vectors & matrices in regression

The general linear regression model,

$$y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_p X_{ip} + \varepsilon_i$$

has the following form in terms of vectors and matrices:

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1p} \\ 1 & x_{21} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & \dots & x_{np} \end{bmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

or,

$$\mathbf{y}_{n\times 1} = \mathbf{X}_{n\times(p+1)} \boldsymbol{\beta}_{(p+1)\times 1} + \boldsymbol{\varepsilon}_{n\times 1}$$

Matrix products in regression

All calculations are based on the sums and sums of squares from the following matrix products (shown for p=1 predictor):

$$\underline{y}'\underline{y} = (y_1, y_2, \dots y_n)\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \underbrace{\sum_{i=1}^{n} y_i^2}_{1\times 1}$$

$$X'X = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} = \underbrace{\begin{bmatrix} n & \sum^{n} x_i \\ \sum^{n} x_i & \sum^{n} x_i^2 \end{bmatrix}}_{2\times 2}$$

$$X'y = \underbrace{\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix}}_{2\times n} \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{n\times 1} = \underbrace{\begin{pmatrix} \sum^{n} y_i \\ \sum^{n} x_i y_i \end{pmatrix}}_{2\times 1}$$

We can represent these all with partitioned matrices:

$$(\mathbf{X} \mid \mathbf{y})'(\mathbf{X} \mid \mathbf{y}) = \left[\begin{array}{c|c} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{y} \\ \hline \mathbf{y}'\mathbf{X} & \mathbf{y}'\mathbf{y} \end{array}\right]$$

Linear combinations of vectors

- Given: vectors $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, $\boldsymbol{x}_3$, ... (same length)
- A linear combination is a weighted sum of the form

$$a\begin{pmatrix} \\ \mathbf{x}_1 \\ \\ \end{pmatrix} + b\begin{pmatrix} \\ \mathbf{x}_2 \\ \\ \end{pmatrix} + c\begin{pmatrix} \\ \mathbf{x}_3 \\ \\ \end{pmatrix}$$

a, b, c: scalars

- e.g., $3\,\boldsymbol{x}_1 + 2\,\boldsymbol{x}_2 - 7\,\boldsymbol{x}_3$
- Why: linear models use linear combinations: $\hat{\mathbf{y}} = \beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2 + \beta_3 \mathbf{x}_3$

Linear combinations of vectors

Simple example:

If $\underline{x}_1 = \begin{pmatrix} 3 \\ 1 \end{pmatrix}$, $\underline{x}_2 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$, $\underline{x}_3 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

then $3\underline{x}_1 + 2\underline{x}_2 - 7\underline{x}_3$

$= 3\begin{pmatrix} 3 \\ 1 \end{pmatrix} + 2\begin{pmatrix} 1 \\ 2 \end{pmatrix} - 7\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 11 \\ 0 \end{pmatrix}$, another vector

Linear independence

- A set of vectors, $\mathbf{x}_1, \mathbf{x}_2, \dots \mathbf{x}_n$ is linearly dependent if:
  1. One $\mathbf{x}_i$ can be expressed as a linear combination of the others; or, equivalently:
  2. There are some scalars, $a_1, a_2, \dots a_n$, not all zero, such that

$$a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \dots + a_n\mathbf{x}_n = \mathbf{0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Otherwise, the vectors are linearly independent.

Why: linear independence → idea of rank of a matrix, # of degrees of freedom

Linear independence: example

eg

$$\begin{array}{cccc} & \text{Verbal} & \text{Math} & \text{Composite} \\ & x_1 & x_2 & x_3 = 2x_1 + x_2 \\ X = & \left[\begin{array}{c} 10 \\ 8 \\ 5 \\ 15 \end{array}\right. & \begin{array}{c} 12 \\ 4 \\ 10 \\ 5 \end{array} & \left.\begin{array}{c} 32 \\ 20 \\ 20 \\ 35 \end{array}\right] \end{array}$$

x_1, x_2, x_3 are linearly dependent

(a) since $x_3 = 2x_1 + x_2$

(b) since $2x_1 + x_2 - x_3 = \mathbf{0}$

$\therefore$ x_3 provides no new information not provided by x_1 & x_2 already (x_3 is redundant, given x_1 & x_2)

When does this arise?

- You include such composite measures
- Ipsatized scores: divide all by the total
- Sample size (N) < # of variables (p)

Consequences: Most analyses will fail, give errors, etc.

Rank of a matrix

The idea of rank of a matrix (or set of vectors) is a fundamental idea in matrix algebra and statistical applications.

- **Def**: rank(**A**) Ξ r (**A**) = # of linearly independent rows (or columns) of $\mathbf{A}_{r \times c}$
- Properties:
  - # linearly independent rows = # linearly independent columns
  - r (**A**) ≤ min(r, c) – rank never greater than smaller dimension
  - r (**A B**) = min[r(**A**), r(**B**)] – rank of product = smaller of separate ranks

- **Geometric idea**: rank = # of dimensions (of a vector space)
- **Statistical idea**: rank = degrees of freedom
  = # of linearly independent variables

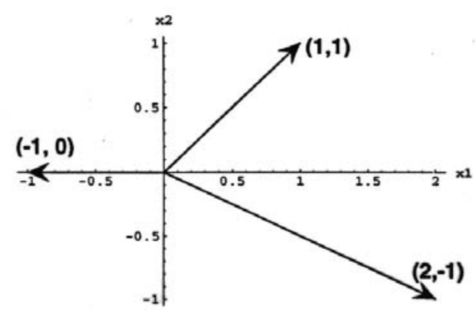
Rank and Dimensionality of Vector Spaces

Row space of a matrix: vector space spanned by rows

Column space of a matrix: vector space spanned by columns

$$A_{(3\times2)} = \begin{array}{c} \begin{array}{cc} x_1 & x_2 \end{array} \\ \begin{pmatrix} 1 & 1 \\ -1 & 0 \\ 2 & -1 \end{pmatrix} \end{array} \begin{array}{c} y_1 \\ y_2 \\ y_3 \end{array}$$

Row space



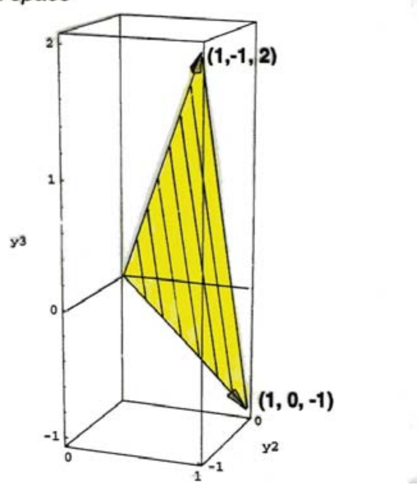
The rows of A define 3 vectors in 2-space, a plane. The columns define 2 vectors in 3-space-- also a plane. Hence, rank(A) = 2.

Rank and Dimensionality of Vector Spaces

rank(A)	Row/Col space
0	point
1	line
2	plane
3	volume
4+	hypervolume

$$A_{(3\times2)} = \begin{array}{cc} x_1 & x_2 \\ \end{array}\quad \begin{pmatrix} 1 & 1 \\ -1 & 0 \\ 2 & -1 \end{pmatrix} \begin{array}{c} y_1 \\ y_2 \\ y_3 \end{array}$$

Column space



Matrix inverse: A^{-1}

Inverse of a number:

- In ordinary arithmetic, division (inverse of multiplication) is essential for solving equations

$$4\,x = 8 \quad \rightarrow \quad x = 8 / 4 = 2$$

- Equally we can regard this is multiplying both sides by the inverse of the constant

$$4\,x = 8 \quad \rightarrow \quad \left(\frac{1}{4}\right) 4\,x = \left(\frac{1}{4}\right) 8 \quad \rightarrow \quad x = 2$$

Matrix inverse: A^{-1}

Inverse of a matrix:

- Division is not defined for matrices, but most square matrices have a matrix inverse, A^{-1}, that plays a similar role in solving equations.
- The inverse of an n x n matrix, A, is defined as a matrix A^{-1} such that its product with A gives the identity matrix:

$$A\ A^{-1} = A^{-1}\ A = I_{(n \times n)}$$

e.g. $D = \begin{pmatrix} 4 & 0 \\ 0 & 3 \end{pmatrix}$ - then $D^{-1} = \begin{pmatrix} 1/4 & 0 \\ 0 & 1/3 \end{pmatrix}$

because $\begin{pmatrix} 4 & 0 \\ 0 & 3 \end{pmatrix}\begin{pmatrix} 1/4 & 0 \\ 0 & 1/3 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$

or $D\ D^{-1} = I$

Matrix inverse: basic properties

- If an inverse, $\mathbf{A}^{-1}$ exists, it is unique
- No inverse exists if $\mathbf{A}_{n \times n} = \mathbf{0}$ (i.e., r(A)=0) or, in general, if r(A) < n
  - → **A** is 'singular'
  - → det(**A**) = |**A**| = 0
- Ordinary inverse defined only for square, non-singular matrices
  - Can also define a 'generalized inverse,' $\mathbf{A}^{-}$, such that $\mathbf{A}\,\mathbf{A}^{-}\,\mathbf{A} = \mathbf{A}$ and $\mathbf{A}^{-}\,\mathbf{A}\,\mathbf{A}^{-} = \mathbf{A}^{-}$

Matrix inverse: 2 x 2

The inverse of a 2 x 2 matrix is easy to calculate:

$$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \rightarrow \mathbf{A}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{|\mathbf{A}|}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

e.g.,

$$\mathbf{A} = \begin{bmatrix} 3 & 2 \\ -1 & 4 \end{bmatrix} \qquad \mathbf{A}^{-1} = \frac{1}{4\times 3 - 1\times(-2)}\begin{bmatrix} 4 & -2 \\ 1 & 3 \end{bmatrix} = \frac{1}{14}\begin{bmatrix} 4 & -2 \\ 1 & 3 \end{bmatrix}$$

Note:

$$\mathbf{AA}^{-1} = \begin{bmatrix} 3 & 2 \\ -1 & 4 \end{bmatrix} \cdot \frac{1}{14}\begin{bmatrix} 4 & -2 \\ 1 & 3 \end{bmatrix} = \frac{1}{14}\begin{bmatrix} 14 & 0 \\ 0 & 14 \end{bmatrix} = \mathbf{I}$$

No inverse if **|A|** = ad – bc = 0, e.g., $A = \begin{bmatrix} 2 & 3 \\ 6 & 9 \end{bmatrix}$

Properties of matrix inverse

1. A^{-1} exists & is unique iff (these are all equivalent)
   (a) $|A| \neq 0$
   (b) A is non-singular
   (c) All rows (cols) of A are linearly independent

2. $I^{-1} = I$ since $I \cdot I = I$

   $(A^{-1})^{-1} = A$ since $(A^{-1})(A^{-1})^{-1} = I$
   $= (A^{-1})(A) = I$

   $(A')^{-1} = (A^{-1})'$

Properties of matrix inverse

3. $(AB)^{-1} = B^{-1}A^{-1}$ since $(AB)(B^{-1}A^{-1})$
   $= ABB^{-1}A^{-1} = AA^{-1} = I$

4. If $D = \begin{pmatrix} d_1 & & 0 \\ & d_2 & \\ 0 & & \ddots d_n \end{pmatrix}$
   & all $d_i \neq 0$ then $D^{-1} = \begin{pmatrix} 1/d_1 & & 0 \\ & 1/d_2 & \\ 0 & & \ddots 1/d_n \end{pmatrix}$

In general, to show or verify that a matrix **K** is the inverse of matrix **L**, show that **K L** = **L K** = **I**

Determinants

For any square matrix, A

$\det(A) \equiv |A| =$ a scalar function of a_{ij}

2x2

$$|A| = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

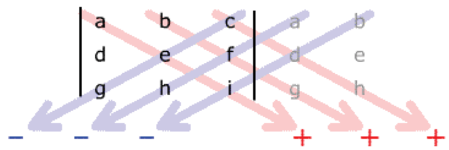
$-$ $\quad$ $+$

each term has 1 element from each row & col

e.g $\begin{vmatrix} 3 & 7 \\ 2 & 8 \end{vmatrix} = 3\cdot 8 - 7\cdot 2 = 10$

Determinants

3 x 3 matrix:
- Copy first 2 cols to the right
- Multiply diagonals
- Add / subtract



= aei + bfg + cdh − ceg − afh − bdi

e.g.

$$\begin{vmatrix} 1 & 3 & 5 \\ 4 & 2 & 3 \\ 1 & 4 & 2 \end{vmatrix} \begin{matrix} 1 & 3 \\ 4 & 2 \\ 1 & 4 \end{matrix}$$

$\overline{1\cdot 2\cdot 5}$ $\overline{4\cdot 3\cdot 1}$ $\overline{2\cdot 4\cdot 3}$

$1\cdot 2\cdot 2$ + $3\cdot 3\cdot 1$ + $5\cdot 4\cdot 4$ +

$$= 4+9+80-10-12-24$$
$$= 93-46 = 47$$

Determinants: cofactors

- General method: expand by cofactors of a given row or column
  - Minor of a_{ij} : M_{ij} = determinant of submatrix removing the *i*th row and *j*th column of **A**.
  - Cofactor of a_{ij} : $C_{ij} = (-1)^{(i+j)} M_{ij}$ (signs alternate)
  - For row i : $\det(A) = a_{i1}C_{i1} + a_{i2}C_{i2} + \cdots a_{in}C_{in}$
  - For col j: $\det(A) = a_{1j}C_{1j} + a_{2j}C_{2j} + \cdots + a_{nj}C_{nj}$

For a_{12}: $\begin{bmatrix} 1 & 0 & 4 \\ -2 & 1 & 8 \\ -1.5 & 6 & 11 \end{bmatrix} \Rightarrow M_{12} = \begin{vmatrix} -2 & 8 \\ -1.5 & 11 \end{vmatrix} \Rightarrow$ $a_{12} \times -1 \times M_{12}$

$0 \times -1 \times (-22+12) = 0$

Determinants: cofactors

Expand by row 1: $\det(A) = a_{11}C_{11} + a_{12}C_{12} + a_{13}C_{13}$

$$M_{11} = \begin{vmatrix} 1 & 8 \\ 6 & 11 \end{vmatrix}$$

$$\begin{bmatrix} 1 & 0 & 4 \\ -2 & 1 & 8 \\ -1.5 & 6 & 11 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 4 \\ -2 & 1 & 8 \\ -1.5 & 6 & 11 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 4 \\ -2 & 1 & 8 \\ -1.5 & 6 & 11 \end{bmatrix}$$

M_{12} M_{13}

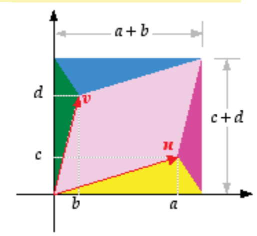
$$+(1)\begin{vmatrix} 1 & 8 \\ 6 & 11 \end{vmatrix} - (0)\begin{vmatrix} -2 & 8 \\ -1.5 & 11 \end{vmatrix} + (-4)\begin{vmatrix} -2 & 1 \\ -1.5 & 6 \end{vmatrix}$$

$$= 1(11-48) - 4(-12+1.5) = -37+42 = \boxed{5}$$

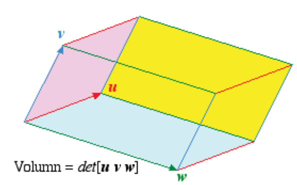
Determinants: geometry

2D: det() = area of parallelogram

$$\det[\mathbf{u} \quad \mathbf{v}] = \det\begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc$$



3D: det() = volume



(What happens if **u**, **v**, **w** are linearly dependent?)

•
•
•

nD: det() = hyper-volume

Correlation matrices:

$$\det\begin{pmatrix} 1 & r_{12} \\ r_{12} & 1 \end{pmatrix} = 1 - r_{12}^2$$

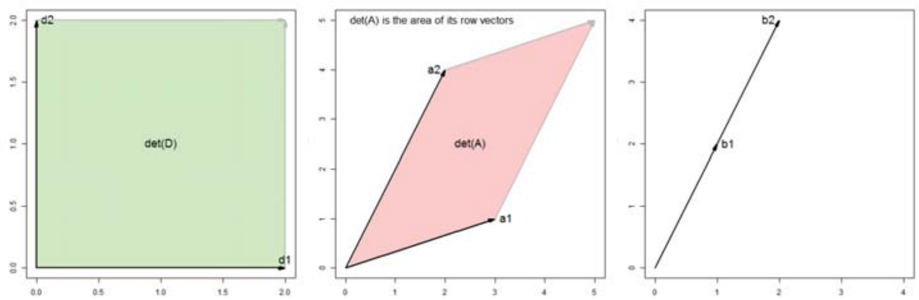
In general: $0 \le \det(\mathbf{R}_{p\times p}) \le 1$

Singular   Uncorrelated, **R=I**

Geometry: 2 x 2

2 x 2 matrices can be visualized by drawing their row (or column) vectors. This illustrates the determinant as the area of the parallelogram

$$D = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \quad |D| = 4 \qquad A = \begin{bmatrix} 3 & 1 \\ 2 & 4 \end{bmatrix} \quad |A| = 10 \qquad B = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \quad |B| = 0$$



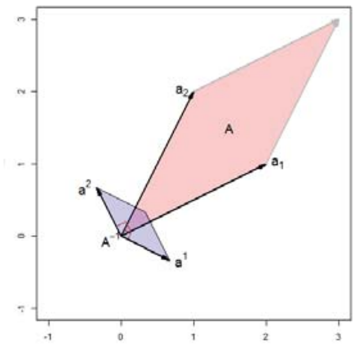
Diagonal matrix   General matrix   Singular matrix

Geometry: Inverse

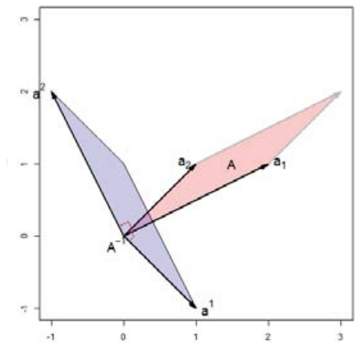
The inverse of a 2 x 2 matrix can be visualized by drawing its row vectors in the same plot. This shows that:

- The shape of $\mathbf{A}^{-1}$ is a 90º rotation of the shape of **A**.
- $\mathbf{A}^{-1}$ is small in the directions where **A** is large; det($\mathbf{A}^{-1}$)= 1/det(**A**)
- The vector a^2 is at right angles to a_1 and a^1 is at right angles to a_2

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad A^{-1} = \frac{1}{3}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$



$$A = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \quad A^{-1} = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}$$



Matrix functions

- Basic matrix functions are provided in base R:
  - `matrix(), c(), rbind(), cbind(), t(), %*%, [,]`
  - `diag(), det(), solve(), crossprod()`
- The **`matlib`** package provides some more:
  - Rank: `R()`, trace: `tr()`, length: `len()`
  - Inverse: `inv()`
  - Many more for linear algebra and vector diagrams

Summary

- Matrices & vectors: shorthand notation
  - Matrix: 2-way table; vector: 1-way collection of #s
  - Algebra:
    - Addition, subtraction: like ordinary arithmetic
    - Multiplication: **a' x** = linear combination; **A x** = set of them
  - Use: represent a linear model: $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$
- Inverse: Matrix "division"
  - Solve linear equations: $\mathbf{A}\,\mathbf{x} = \mathbf{b} \rightarrow \mathbf{x} = \mathbf{A}^{-1}\,\mathbf{b}$
  - statistical models: inverse of covariance matrix → std.errors
- Determinant: "size" of a square matrix
  - $|\mathbf{A}| = 0$ → "singular," no inverse, can't solve
  - Rank = # linearly independent rows, cols, equations