Mathematical Preliminaries (Vector & Matrix Algebra)

Nagiza F. Samatova, samatova@csc.ncsu.edu
Professor, Department of Computer Science
North Carolina State University

Senior Scientist, Computer Science & Mathematics Division
Oak Ridge National Laboratory

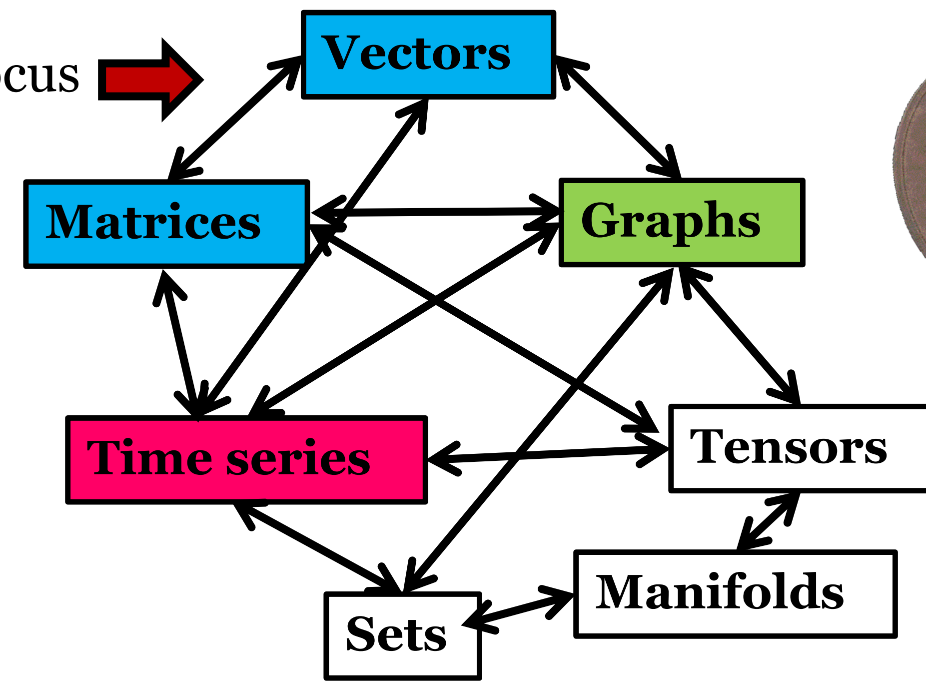
Mathematical Preliminaries

VECTOR & MATRIX ALGEBRA

Recap: Data Mining Process

Application → Data → Questions → Data Objects + Features → **Mathematical Data Representation (Data Model)**

Today's focus



Not one hat fits all

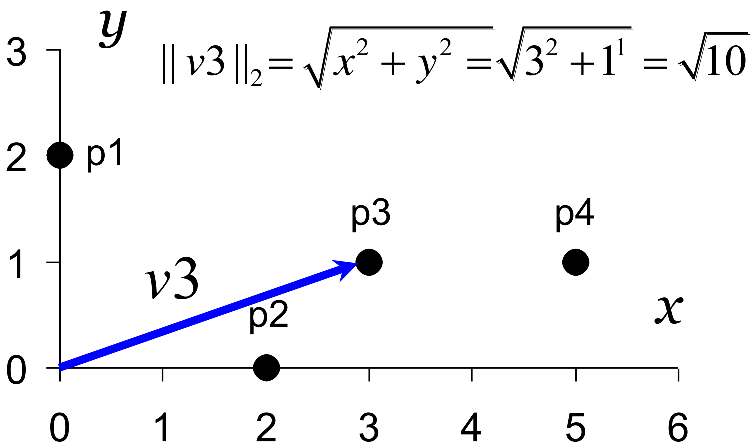
More than one models are needed

Models are related

Vectors in Low- and High-dimensional Spaces

Points in 2-dimensional space

$$\| v3 \|_2 = \sqrt{x^2 + y^2} = \sqrt{3^2 + 1^1} = \sqrt{10}$$



Data Points in 2-d

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

Do not mix with *length(v)* in R:
- number of vector components, *d*

Point ⟷ Vector

$$\boxed{p3 = (x, y) \leftrightarrow v3 = (x, y)}$$

Vector has:
- The origin (0,0)
- The direction
- The length/norm: ||v||

In ***d***-dimensional space:

$$p = (p_1, p_2, \ldots, p_d) \in R^d \quad \leftrightarrow$$
$$v = (v_1, v_2, \ldots, v_d) \in R^d$$

Vector length/norm (e.g. L_2-norm):

scalar

$$\boxed{\| v \|_2 = \sqrt{\sum_{k=1}^{d} (v_k)^2} \in R}$$

Normalized Vector (L_2-norm=1):

$$\boxed{u = \frac{v}{\| v \|}}$$

Ex #1: Vector Norm

Consider the vector in a two-dimensional space:

$$\boldsymbol{v} = (\mathbf{1}, -\mathbf{2}) \in \mathbb{R}^{\mathbf{2}}$$

a. What is the length, i.e., the L_2 −norm of this vector? Show calculations by hand. Validate the result by showing the R code that does the same.

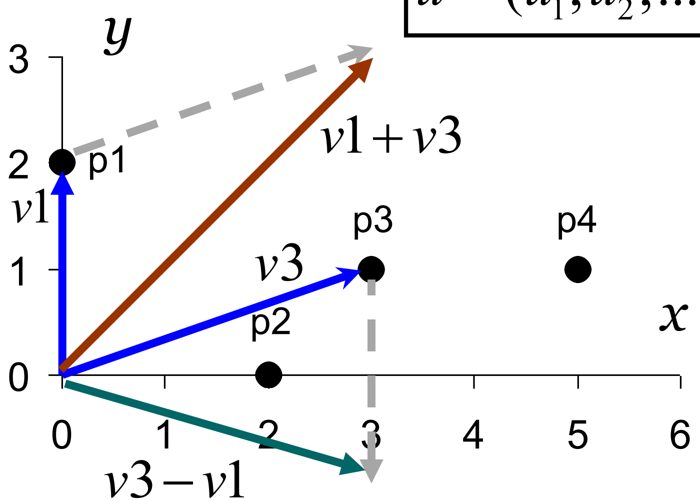
$$||\boldsymbol{v}|| =$$

b. Normalize this vector to the unit length? Show calculations by hand. Validate the result by showing the R code that does the same.

$$||\boldsymbol{v_n}|| =$$

Some Vector Operations

$$u = (u_1, u_2, \ldots, u_d) \in R^d \text{ and } v = (v_1, v_2, \ldots, v_d) \in R^d$$



Scaling:

vector

$$\alpha \cdot u = (\alpha \cdot u_1, \ldots, \alpha \cdot u_d) \in R^d$$

Vector Sum:

vector

$$u + v = (u_1 + v_1, \ldots, u_d + v_d) \in R^d$$

Vector Difference:

vector

$$u - v = (u_1 - v_1, \ldots, u_d - v_d) \in R^d$$

Data Points in 2-d

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

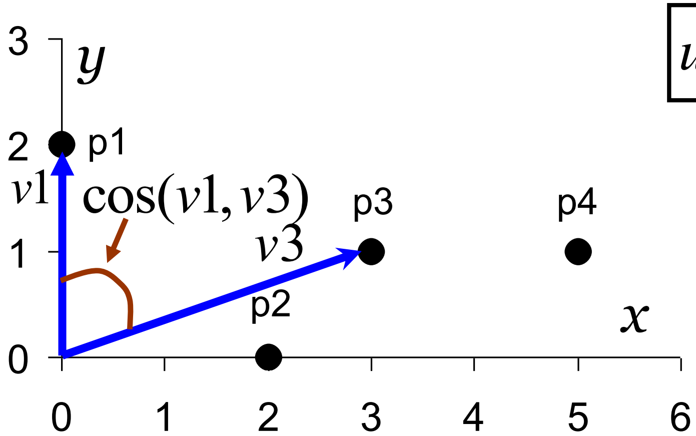
Scalar Product of Two Vectors:

scalar

$$(u, v) = u_1 \cdot v_1 + \ldots + u_d \cdot v_d \in R$$

- *v = c (5,1,3); u = c(2,5,5)*
- *u+v; u-v;*
- *u*v; 2*v;*

Cosine between Two Vectors



Data Points in 2-d

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

$$\| v1 \| = \sqrt{4} = 2$$

$$\| v3 \| = \sqrt{10}$$

$$(v1, v3) = 3 \cdot 0 + 1 \cdot 2 = 2$$

$$\cos(v1, v3) = \frac{2}{2 \cdot \sqrt{10}} = \frac{1}{\sqrt{10}}$$

$$\boxed{u = (u_1, u_2, \ldots, u_d) \in R^d \text{ and } v = (v_1, v_2, \ldots, v_d) \in R^d}$$

Scalar Product of Two Vectors:

scalar

$$\boxed{(u, v) = u_1 \cdot v_1 + \ldots + u_d \cdot v_d \in R}$$

Vector length/norm (e.g. L_2-norm):

scalar

$$\boxed{\| v \|_2 = \sqrt{\sum_{k=1}^{d} (v_k)^2} \in R}$$

Cosine between Two Vectors:

scalar

$$\boxed{\cos(u, v) = \frac{(u, v)}{\| u \| \cdot \| v \|} \in R}$$

Orthogonal Vectors:

$$u \perp v \Rightarrow \cos(u, v) = 0 \Rightarrow (u, v) = 0$$

$$u = (1, 1), v = (1, -1)$$

Ex #2: Scalar/Inner Product & Cosine

Consider two vectors in a two-dimensional space:

$$\boldsymbol{v} = (\mathbf{1}, -\mathbf{2}), \boldsymbol{u} = (\mathbf{2}, \mathbf{1}) \in \mathbb{R}^{\mathbf{2}}$$

a. What is the scalar product (aka inner product) of these two vectors? Show calculations by hand. Validate the result by showing the R code that does the same. Is scalar product symmetric, i.e. $(v, u) = (u, v)$?

$$(\boldsymbol{v}, \boldsymbol{u}) =$$

$$(\boldsymbol{u}, \boldsymbol{v}) =$$

b. What is the value of $\cos(u, v)$? Show calculations by hand. Validate the result by showing the R code that does the same. Are these two vectors perpendicular, i.e., angle is 90°?

$$\boldsymbol{cos}(\boldsymbol{u}, \boldsymbol{v}) =$$

Ex #3: Scalar/Inner Product & Cosine

Consider two vectors in a four-dimensional space:

$$\boldsymbol{v} = (\mathbf{1}, -\mathbf{2}, \mathbf{1}, -\mathbf{2}), \boldsymbol{u} = (\mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}) \in \mathbb{R}^{\mathbf{4}}$$

a. What is the scalar product (aka inner product) of these two vectors? Show calculations by hand. Validate the result by showing the R code that does the same. Is scalar product symmetric, i.e. $(v, u) = (u, v)$?

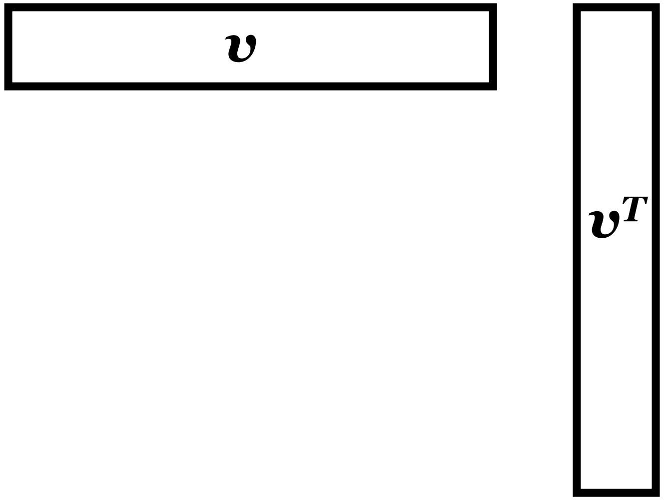
$$(\boldsymbol{v}, \boldsymbol{u}) =$$

$$(\boldsymbol{u}, \boldsymbol{v}) =$$

b. What is the value of $\cos(u, v)$? Show calculations by hand. Validate the result by showing the R code that does the same. Are these two vectors perpendicular, i.e., angle is 90°?

$$\boldsymbol{cos}(\boldsymbol{u}, \boldsymbol{v}) =$$

Vector Transpose (v^T)

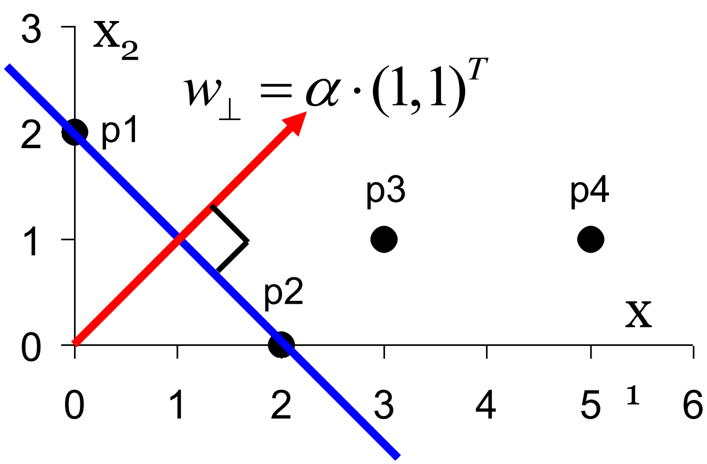


- *v = c (5,1,3);*
- *vt = t (v);*
- *help (t)*

Lines, Planes, Hyperplanes, Normal Vectors

Line in 2-dimensions:

$$\boxed{\begin{array}{l} y = ax + b, \text{ or equivalently} \\ l : a_1 x_1 + a_2 x_2 + b = 0 \end{array}}$$



$$\boxed{\begin{array}{l} l : x_1 + x_2 - 2 = 0 \\ w_\perp = (1,1)^T \text{ and } b = -2 \end{array}}$$

Line, l ⟷ **Normal Vector** (orthogonal to l)

$$\boxed{l \leftrightarrow w_\perp = (a_1, a_2)^T}$$

$$\boxed{\begin{array}{l} x = (x_1, x_2) \\ w_\perp = (a_1, a_2)^T \\ l : x \cdot w_\perp + b = 0 \end{array}}$$

Plane in 3-dimensions:

$$\boxed{a_1 x_1 + a_2 x_2 + a_3 x_3 + b = 0}$$

Hyper-plane in *d*-dimensions:

$$\boxed{a_1 x_1 + a_2 x_2 + \ldots + a_d x_d + b = 0}$$

$$\boxed{l \leftrightarrow w_\perp = (a_1, a_2, \ldots, a_d)^T}$$

Ex #4: Normal Vector to a Line

Consider the line in a 2-dimensional space:

$$\boldsymbol{l}\colon\ \boldsymbol{x_1} - \boldsymbol{x_2} + \mathbf{2} = \mathbf{0} \in \mathbb{R}^{\mathbf{2}}$$

a. What is the normal vector $\boldsymbol{w}_{\perp}$ for the line, i.e. the perpendicular vector to this line?

$$\boldsymbol{w}_{\perp}(\boldsymbol{l}) = ?$$

b. What is the value of the intercept b for this line?

$$\boldsymbol{b} = ?$$

c. Choose any point p that lies on this line and give its coordinates:

$$\boldsymbol{p} = (\boldsymbol{x_1} = \quad , \boldsymbol{x_2} = \quad) \in \boldsymbol{l}$$

d. Show (by manual calculations) that the following is true:

$$(\boldsymbol{p}, \boldsymbol{w}_{\perp}) + \boldsymbol{b} = \mathbf{0}$$

Ex #5: Normal Vector to a Plane

Consider the plane in a 3-dim. space:

$$\boldsymbol{\alpha}: \boldsymbol{x_1} + \boldsymbol{x_2} - \boldsymbol{x_3} - \mathbf{1} = \mathbf{0} \in \mathbb{R}^{\mathbf{3}}$$

a. What is the normal vector $\boldsymbol{w}_\perp$ for the plane, i.e. perpendicular vector to this plane?

$$\boldsymbol{w}_\perp(\boldsymbol{\alpha}) = ?$$

b. What is the value of the intercept b for this plane?

$$\boldsymbol{b} = ?$$

c. Choose any point p that lies on this plane and give its coordinates:

$$\boldsymbol{p} = (\boldsymbol{x_1} = \quad, \boldsymbol{x_2} = \quad, \boldsymbol{x_3} = \quad) \in \boldsymbol{\alpha}$$

d. Show (by manual calculations) that the following is true:

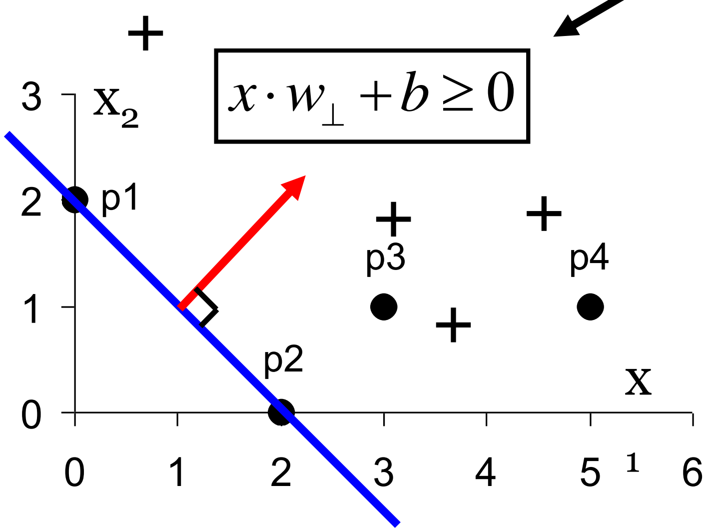
$$(\boldsymbol{p}, \boldsymbol{w}_\perp) + \boldsymbol{b} = \mathbf{0}$$

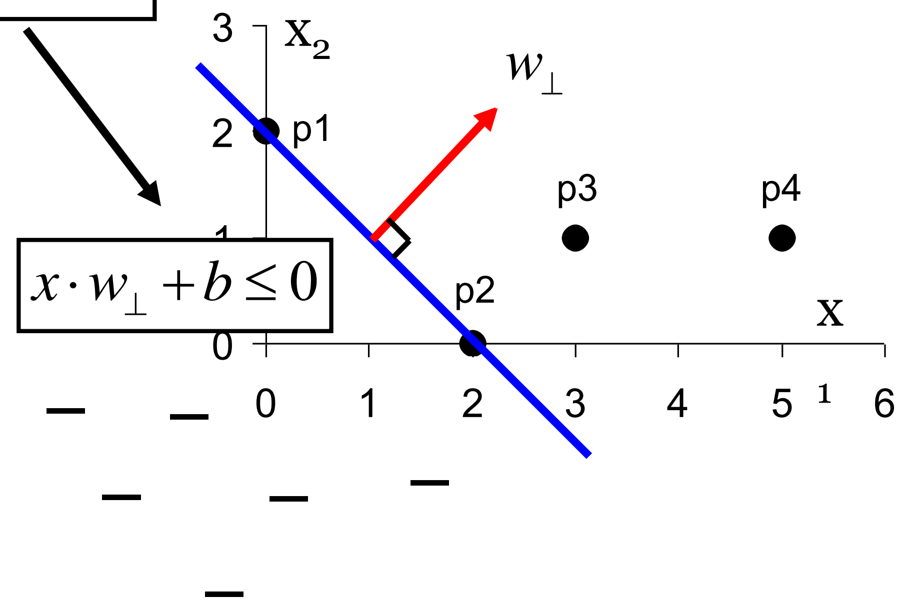
Half-Planes, Half-Spaces, Half-Hyperspaces

$$x = (x_1, x_2, \ldots, x_d)$$

$$w_\perp = (a_1, a_2, \ldots, a_d)^T$$

$$x \cdot w_\perp + b = 0$$





$$x = p3 = (3,1)$$

$$w_\perp = (1,1)^T \text{ and } b = -2$$

$$p3 \cdot w_\perp + b = 3 \cdot 1 + 1 \cdot 1 - 2 = 2 \geq 0$$

Ex #6: Half-Planes

Consider the plane in a 3-dim. space:

$$\boldsymbol{\alpha}\text{: } \boldsymbol{x_1 + x_2 - x_3 - 1 = 0} \in \mathbb{R}^3$$

a. Give coordinates of any point p that lies in the **positive half-plane** of this plane:

$$\boldsymbol{p} = (?\,,?\,,?\,) \in \boldsymbol{\alpha}$$

b. Show (by manual calculations) that the following is true:

$$(\boldsymbol{p}, \boldsymbol{w}_\perp) + \boldsymbol{b} > \boldsymbol{0}$$

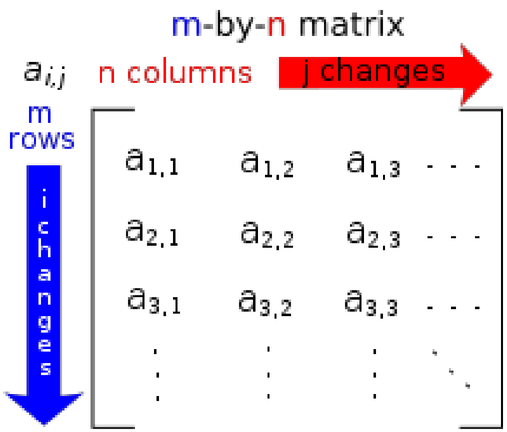
d. Give coordinates of any point q that lies in the **negative half-plane** of this plane:

$$\boldsymbol{q} = (?\,,?\,,?\,) \in \boldsymbol{\alpha}$$

e. Show (by manual calculations) that the following is true:

$$(\boldsymbol{q}, \boldsymbol{w}_\perp) + \boldsymbol{b} < \boldsymbol{0}$$

Matrix and its Transpose



$$\boxed{(A^T)_{i,j} = A_{j,i}} \qquad \boxed{(A^T)^T = A}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 0 & -6 & 0 \end{bmatrix}^T = \begin{bmatrix} 1 & 0 \\ 2 & -6 \\ 3 & 0 \end{bmatrix}$$

- A = *matrix (c (1,0,2,-6,3,0), nrow=2, ncol=3);*
- *A;*
- *B = t (A);*
- *B;*
- *t (B);*
- *help (t)*

Ex #7: Transpose of the Matrix

Consider the following 3-by-2 matrix:

$$\mathbf{A}=\begin{bmatrix} \mathbf{1} & \mathbf{-2} \\ \mathbf{0} & \mathbf{3} \\ \mathbf{2} & \mathbf{-1} \end{bmatrix}$$

a. What is the value of $\boldsymbol{A}[\mathbf{3},\mathbf{2}] =$?

b. Show its transpose matrix and validate with R code: $\boldsymbol{A}^{\boldsymbol{T}} =$

c. What is the value of $\boldsymbol{A}^{\boldsymbol{T}}[\mathbf{1},\mathbf{2}] =$?

d. If the matrix had m rows and n columns, then how many rows the transpose matrix will have?

Some Matrix Operations: Element-by-Element

$$\dim(A) = \dim(B) = m \times n$$

$$(c \cdot A)_{i,j} = c \cdot A_{i,j}$$

$$(A \pm B)_{i,j} = A_{i,j} \pm B_{i,j}$$

$$(A \otimes B)_{i,j} = A_{i,j} \cdot B_{i,j}$$

$$(A / B)_{i,j} = A_{i,j} / B_{i,j}$$

```
A=matrix(c(54,49,49,41,26,43,49,50,58,71),nrow=5,ncol=2))
B=matrix(c(1:10), nrow=5, ncol=2))
```

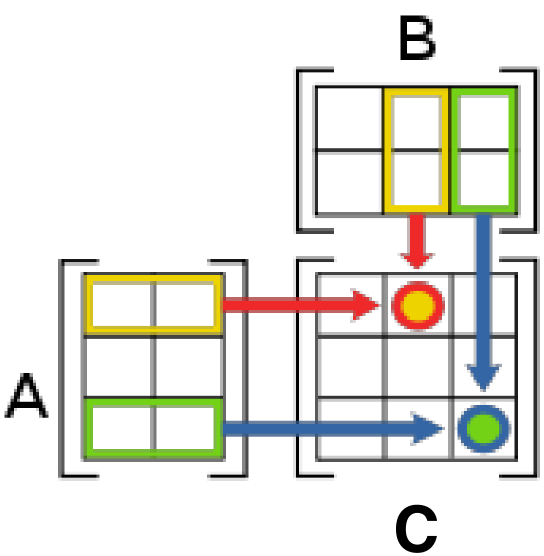
To perform element-by-element ops:

```
2*A+3; A+B; A-B; A*B; A/B;
```

Matrix-Matrix Multiplication

$\dim(A) = m \times n$ $\dim(B) = n \times k$

$C = A * B$ $\dim(C) = m \times k$



$$(A*B)_{i,j} = A_{i,1}B_{1,j} + A_{i,2}B_{2,j} + \ldots + A_{i,n}B_{n,j} = \sum_{r=1}^{n} A_{i,r}B_{r,j}$$

$$\begin{bmatrix} 1 & 0 & 2 \\ -1 & 3 & 1 \end{bmatrix} \times \begin{bmatrix} 3 & 1 \\ 2 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 5 & 1 \\ 4 & 2 \end{bmatrix}.$$

$\underline{2} \times 3$ $3 \times \underline{2}$ $\underline{2} \times \underline{2}$

In R:

```
C = A%*%B;
```

Ex #8: Matrix-Matrix Multiplication

1. Generate in R a 3-by-3 matrix A filled with one's everywhere but the diagonal; and with 3's on the diagonal.
2. Generate in R a 3-by-2 matrix B filled with two's.

a. Multiply in R matrix A by matrix B and print the resulting matrix C:

$$\boldsymbol{C} = \boldsymbol{AB} =$$

b. What is the size of this new matrix **C**, i.e. number of rows and cols?

c. Can you multiply matrix B by A to get matrix D (why or why not):

$$\mathbf{D} = \boldsymbol{BA} =$$

d. Show with manual calculations how you will get the value of:

$$\boldsymbol{C}[\mathbf{2}, \mathbf{2}] =$$

Ex #9: Projection Matrix

1. Generate in R a 4-by-2 matrix A and plot its 4 rows as points in 2-dim.
2. Generate a 2-by-2 matrix with diagonal elements as one's and off-diagonal matrix as zero's (aka ***identity*** matrix, I).

a. Multiply in R matrix A by matrix I and print the resulting matrix C:

$$\boldsymbol{C} = \boldsymbol{A}\,\boldsymbol{I} =$$

b. Set the $\boldsymbol{I}[\mathbf{2},\mathbf{2}]$ element to zero and assign the new matrix to P.

c. Multiple matrix A by the modified matrix I to get matrix D:

$$\mathbf{D} = \boldsymbol{A}\,\boldsymbol{P} =$$

d. Add the rows of matrix D as four points in 2-dim. to your original plot of A.
Do you observe that these new points are projections of the original points? What axis are the points of A projected to in D?

e. How will you modify the identity matrix I to project the points of A on the other axis?

Advanced Topics: Optional

Inverse of a Square Matrix, nrow(A)=ncol(A)

Identity Matrix, I_n

$$I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Determinant, ***det(A)***, $|A|$

scalar: $\det\begin{pmatrix} a & b \\ c & d \end{pmatrix} = ad - bc$

```
A = matrix (rnorm(16), nrow=4,ncol=4);
IA = solve (A);
help (solve);
```

Matrix Inverse, A^{-1}

$$\boxed{A * A^{-1} = A^{-1} * A = I}$$

$$A^{-1} \text{ exists} \Leftrightarrow \det(A) \neq 0$$

2-by-2 **Matrix Inverse**

$$A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

n-by-n **Matrix Inverse**

- LU-factorization
- Gaussian elimination
- Gauss-Jordan elimination

Mathematical Preliminaries

MATRIX DECOMPOSITION & TRANSFORMATIONS

Linear Transformation Matrix

Matrix-based Transformation of Vectors

$$v_{old} \xrightarrow[\text{matrix, } A]{} v_{new}$$

- **Scaling Matrix**
- **Reflection Matrix**
- **Rotation Matrix**
- **Projection Matrix**

Notation

$$\boldsymbol{u} = [u_1, u_2, ..., u_p] - \text{ row vector}$$

$$\boldsymbol{v} = \begin{bmatrix} v_1 \\ ... \\ v_m \end{bmatrix} - \text{ column vector}$$

$$\boldsymbol{A} = \boldsymbol{A}_{m\times p} = \begin{bmatrix} a_{11} & ... & a_{1p} \\ ... & ... & ... \\ a_{m1} & ... & a_{mp} \end{bmatrix} - m \times p \text{ matrix}$$

$$\boldsymbol{I} = \boldsymbol{I}_{m\times m} = \begin{bmatrix} 1 & 0 & ... & 0 \\ 0 & 1 & ... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & 0 & 1 \end{bmatrix} - \text{ identity matrix}$$

Scaling Matrix

Row vectors:

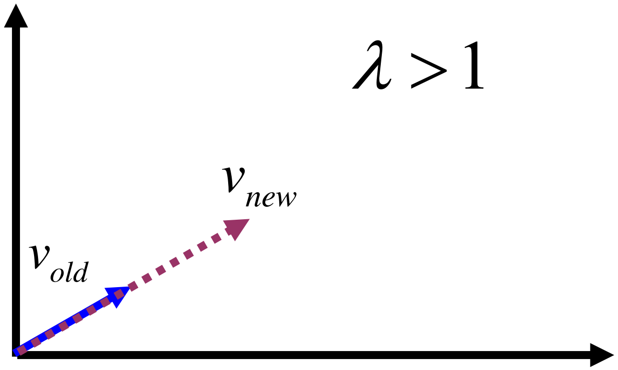
$$v_{old} \in R^p \xrightarrow[\text{scalar, } \lambda \in R^+]{\text{matrix, } \boldsymbol{A}} v_{new} = \lambda \cdot v_{old} \in R^p$$

$$\boldsymbol{A}_\lambda = \lambda \cdot \boldsymbol{I}_{p\times p} = \begin{bmatrix} \lambda & 0 & \dots & 0 \\ 0 & \lambda & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \lambda \end{bmatrix} - \text{scaling matrix}$$

$$v_{new} = v_{old} \cdot \boldsymbol{A} = v_{old} \cdot \lambda \cdot \boldsymbol{I}_{p\times p}$$

- **Unchanged:**
  - **Direction of a vector**
- **Changed:**
  - **Vector norm/length**

$$\| v_{new} \| = \lambda \cdot \| v_{old} \|$$



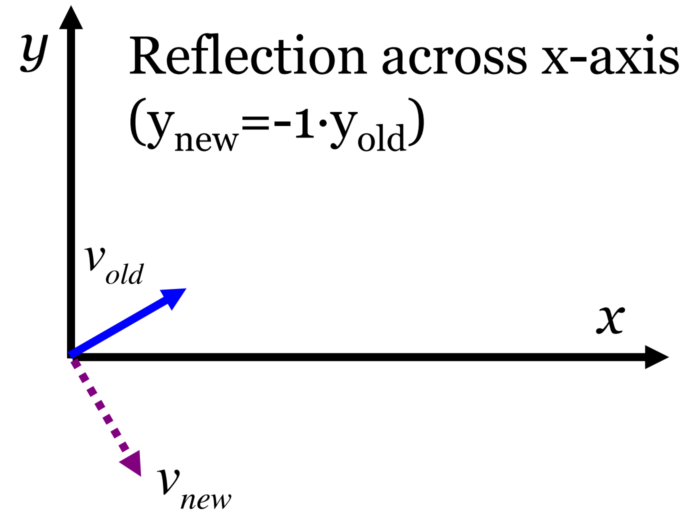
Reflection Matrix

Row vectors:

$$v_{old} \in R^p \underset{\text{matrix, } A}{\longrightarrow} v_{new} = v_{old} \cdot A \in R^p$$

- **Changed:**
  - **Direction of a vector**
  - **Reflects across >=1 axis**
- **Unchanged:**
  - **Vector norm/length**

$$\boldsymbol{A} = \boldsymbol{I}'_{p \times p} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 1 \end{bmatrix} - \text{reflection matrix; some elements are -1}$$



$$v_{new} = v_{old} \cdot A$$

Equivalent to: multiplying one or more vector components by -1

Rotation Matrix

Row vectors:

$$v_{old} \in R^p \underset{\substack{\text{matrix, } \boldsymbol{A} \\ \boldsymbol{det(\ A\ )=1} \\ \boldsymbol{A}^T = \boldsymbol{A}^{-1}}}{\longrightarrow} v_{new} = v_{old} \cdot \boldsymbol{A} \in R^p$$

- **Changed:**
  - **Direction of a vector**
- **Unchanged:**
  - **Vector norm/length**

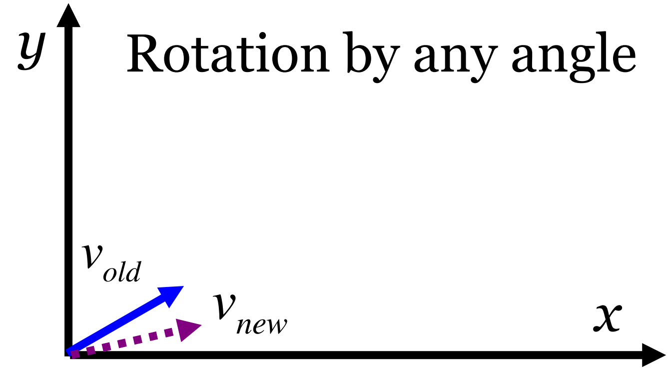
$$\boldsymbol{A} = \boldsymbol{A}_{p\times p} = \begin{bmatrix} a_{11} & \dots & a_{1p} \\ \dots & \dots & \dots \\ a_{p1} & \dots & a_{pp} \end{bmatrix} - p \times p \text{ orthogonal matrix}$$

$$\boldsymbol{A}^T = \boldsymbol{A}^{-1} - \text{orthogonal matrix}$$

$$\det(\boldsymbol{A}) = 1$$

Example: *p*=2

$$A(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} - \text{clockwise rotation by } \theta$$



Projection Matrix

Row vectors:

$$v_{old} \in R^{p} \xrightarrow[\text{matrix, } \boldsymbol{A}]{} v_{new} = v_{old} \cdot \boldsymbol{A} \in R^{d},\ d < p$$

- **Changed:**
  - **Dimensionality of a vector**
  - **Direction of a vector**
  - **Vector norm/length**