Matrix theory and linear algebra

Matrix Theory and Linear Algebra

- Matrices can be used to represent samples with multiple attributes in a compact form
- Matrices can also be used to represent linear equations in a compact and simple fashion
- Linear algebra provides tools to understand and manipulate matrices to derive useful knowledge from data

Matrices for data science: Data representation

- Usually matrices are used to store and represent the data on machines
- Matrix is a very natural approach for organizing data
- In general, data is organized in the following fashion
  - Rows represent samples
  - Columns represent the values of the variables (or attributes)
  - It is also possible to use rows for variables and columns for samples
  - However, we will stick to rows as samples and columns as variables in all of the material that will be presented

Data representation: Examples

- A real life example
  - Consider a reactor which needs to be controlled using multiple attributes from various sensors like Pressure (Pa), Temperature (K), Density (gm/m^3) etc.
  - Independently, the sensors have generated 1,000 data points
  - This complete set of information is contained in

$$
\begin{array}{c c}
 & \begin{array}{ccc} P & T & \rho \end{array} \\
\begin{array}{c} 1 \\ \vdots \\ 1000 \end{array} & \begin{bmatrix} 300 & 300 & 1000 \\ \vdots & \vdots & \vdots \\ 500 & 1000 & 5000 \end{bmatrix}
\end{array}
$$

Data representation: Examples

- Example 2:

$$X = [1,2,3]^T$$
$$Y = [2,4,6]^T$$

- X and Y are vectors pertaining to some attributes
- We define the A matrix using a column bind of X and Y thus representing data in a matrix format (the code for the same is attached)

R Code

```
x=c(1,2,3)
y=c(2,4,6)
A=cbind(x,y)
print(A)
```

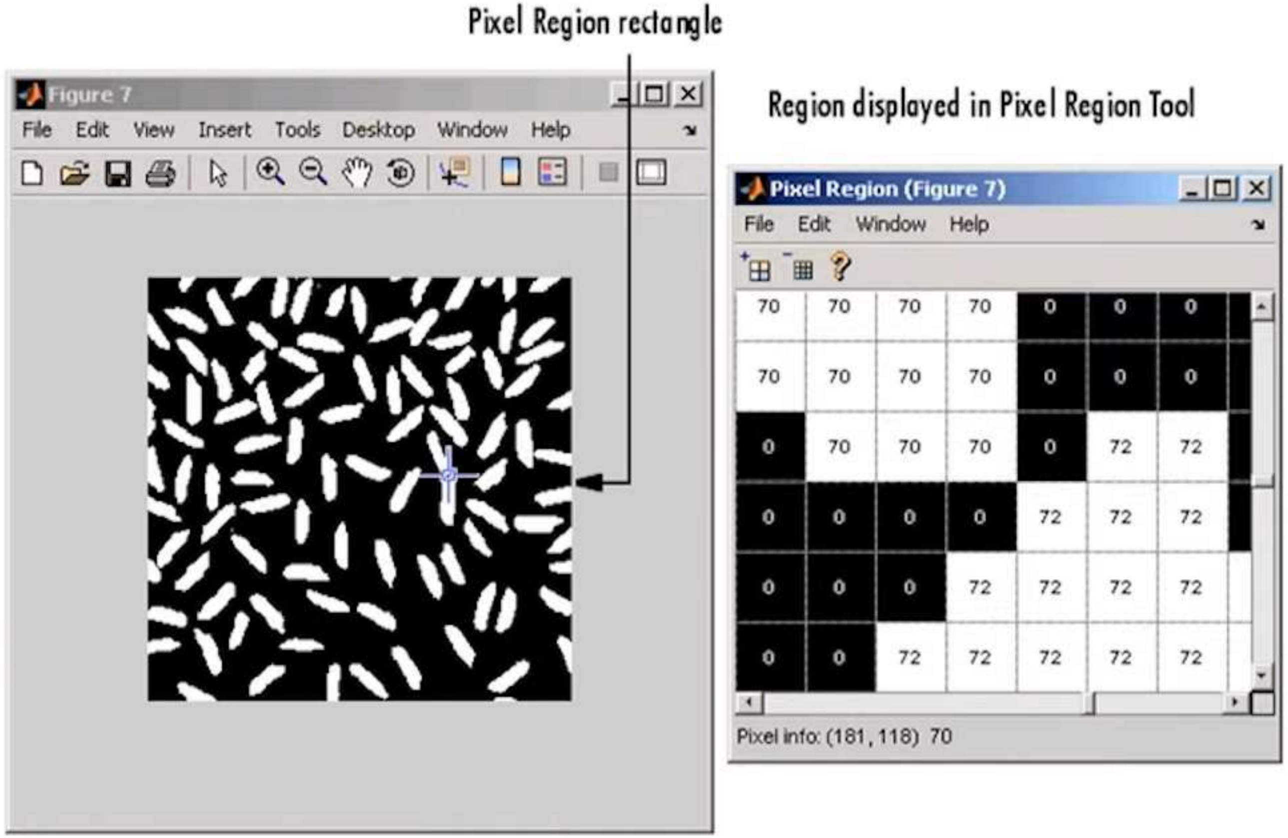
$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \end{bmatrix}$$

Output

```
> print(A)
     x y
[1,] 1 2
[2,] 2 4
[3,] 3 6
```

Data representation: Examples

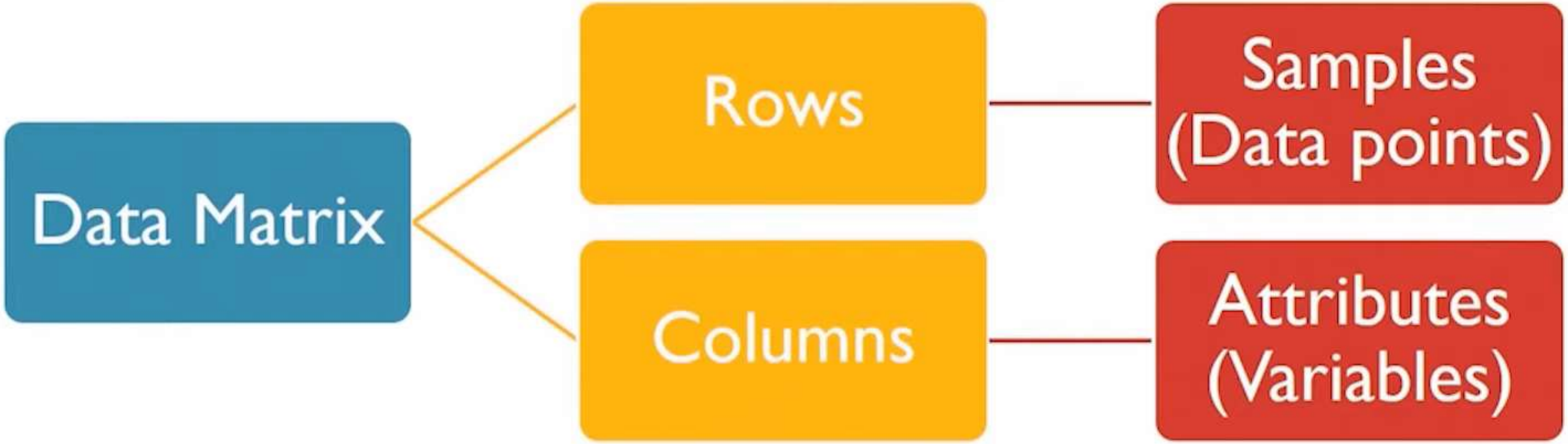
- The simplicity in representation will become apparent when the image below is considered



Data representation: Examples

- Storing
  - The image is stored in the machine as a large matrix of pixel values across the image.
  - Thus, storing the pixel value matrix is equivalent to storing the image for the machine
- Identification
  - Several machine learning algorithms are deployed in order to "teach" the machine how to identify a particular image.
  - Linear algebra and matrix operations are at the heart of these machine learning algorithms.

Data as matrix: Summary



IDENTIFICATION OF INDEPENDENT ATTRIBUTES

Further analysis

- Now that we can represent the data into a matrix format, we ask the following questions
  - Are all the attributes in the data matrix relevant/ important?
  - Is there any method which can identify if some attributes are related to the other attributes?
  - If yes, how do we identify the linear relationship?
  - Can we use this to reduce the size of the data matrix?

Identification of independent attributes: Example

- Consider the ideal reactor example with multiple (say, 4) attributes like Pressure, Temperature, Density, Viscosity, etc. with 500 samples.
- Thus we have a 500 X 4 matrix such that

$$A = [P\ T\ D\ \eta]$$

- P, T, D and η are vectors of 500 samples from the pressure, temperature, density and viscosity sensors.
- How does one identify the number of independent attributes?

Identification of independent attributes: Example

- Domain knowledge

$$D \sim f(P, T)$$

- Thus, in some sense **D** is a function of **P** and **T**
- Implying that at least one attribute is dependent on the others
- This variable can be calculated as a linear combination of the other variables
- The physics of the problem helps us identify the relationship in the data matrix
- We now ask if the data itself will help us identify these relationships

Number of independent attributes: Rank of a matrix

- Let us assume that we have many more samples than attributes for now
- Is there any approach which can be used to identify the number of linear relationships between the attributes purely using data?
- This is addressed by the concept of the **rank** of the matrix.
- **Rank** of a matrix refers to the number of linearly independent rows or columns of the matrix
- The rank of a matrix can be found using the rank command: rank(A)

Rank of a matrix: Example 2

- Consider another example

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 0 \\ 3 & 6 & 0 \end{bmatrix}$$

- We observe that
  - (Col. 2)=2 x (Col. 1)
  - (Col. 3) is independent
- Thus, the rank of this matrix is 2

R Code

```
A=matrix(c(1,2,3,2,4,6,1,0,0),ncol=3,byrow=F)
library(pracma)
Rank(A)
```

Output

```
> Rank(A)
[1] 2
```

Rank: Advantages and summary

Rank

- Work with reduced set of variables
- Dependent attributes can be calculated if they are from the same data generation process
- Independent of the size of the dataset if the data is from the same data generation process

IDENTIFICATION OF LINEAR RELATIONSHIPS AMONG ATTRIBUTES

Linear relationships among attributes

- Now that we have identified the number of linearly independent attributes:
  - How does one identify those linear relations among the attributes?
- Such questions are addressed by the linear algebraic concepts of null space and nullity

Null space for data science

- The null space of a matrix **A** consists of all vectors $\boldsymbol{\beta}$ such that $\boldsymbol{A\beta} = \mathbf{0}$ and $\boldsymbol{\beta} \neq \mathbf{0}$
- Nullity of a matrix is the number of vectors in the null space of the given matrix
- The size of the null space of a matrix provides us with the number of linear relations among the attributes
- And the null space vectors $\boldsymbol{\beta}$ are useful to identify these linear relationships

Null space : general description

- Let us suppose
- $A = \begin{bmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{bmatrix}$ is a data matrix and there is one vector in the null space of A, i.e, $\beta = [\beta_1 \ \ldots \beta_n]^T$, then as per the definition, β satisfies all the equations given below

- $x_{11}\beta_1 + x_{12}\beta_2 + \cdots x_{1n}\beta_n = 0$

$$\vdots$$

- $x_{m1}\beta_1 + x_{m2}\beta_2 + \cdots x_{mn}\beta_n = 0$

Null space: The idea

- Notice that if $\boldsymbol{A\beta} = \mathbf{0}$, every row of A when multiplied by $\boldsymbol{\beta}$ goes to zero
- This implies that variable values in each sample (represented by a row) behave the same
- This helps in identifying the linear relationships in the attributes
- Every null space vector corresponds to one linear relationship
- This idea is demonstrated further using examples

Rank nullity theorem

- Consider the data matrix A with the null space and nullity as defined before
- The rank- nullity theorem helps us to relate the nullity of the data matrix to the rank and the number of attributes in the data
- According to the rank-nullity theorem

Number of equations

Number of independent variables

Total number of variables

Summary till now

Data Matrix

- The available data is expressed in the form of a data matrix
- This data matrix is further used to do the necessary operations

Null Space

- Defined as a collection of vectors satisfying $A\beta = 0$
- Helps in identifying the linear relationships between the attributes directly

Nullity

- Nullity is the size of the null space of the data matrix
- Useful to identify the number of linear relationships in the attributes
- Rank- Nullity theorem

Null space: An Example

- Consider the matrix A with attributes $\{x_1, x_2\}$

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

Number of columns in A =2

Rank of A =2

Thus, nullity =0

- This implies that the null space of the matrix A does not contain any vectors
- Thus we can claim that all the attributes are linearly independent

Console output

```
> A
     [,1] [,2]
[1,]    1    2
[2,]    3    4
[3,]    5    6
```

Console output

```
>print(columns)
[1] 2
> print(rank)
[1] 2
> print(nullity)
[1] 0
```

R Code

```
A=matrix(c(1,3,5,2,4,6),ncol=2, byrow=F)
columns=ncol(A)
library(pracma)
rank=Rank(A)
nullity=columns-rank
```

Null space: Another example

- Now consider A with attributes $\{x_1, x_2, x_3\}$ such that

$$\begin{bmatrix} 1 & 2 & 0 \\ 2 & 4 & 0 \\ 3 & 6 & 1 \end{bmatrix}$$

Number of columns in A =3

Rank of A =2

Thus, nullity =1

- Thus, we need to identify the vectors in the null space of A which is non-zero in this case

R Code

```
A=matrix(c(1,2,3,2,4,6,0,0,1),ncol=3, byrow=F)
columns=ncol(A)
library(pracma)
rank=Rank(A)
nullity=columns-rank
```

Console output

```
> columns
[1] 3
> rank
[1] 2
> nullity
[1] 1
```

Null space: Further Example

$$A\boldsymbol{\beta} = 0$$

$$\begin{bmatrix} 1 & 2 & 0 \\ 2 & 4 & 0 \\ 3 & 6 & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

- Thus we obtain,

$$b_1 + 2b_2 = 0$$
$$b_3 = 0$$

- The null vector is $\boldsymbol{B} = [b_1 \ \ b_2 \ \ b_3\ ]^T = [-2b_2 \ \ b_2 \ \ 0]^T = k[-2\ 1\ 0]^T$
- We see that we obtain a direct linear relationship between the attributes of A using null space and rank-nullity theorem
- The same concept can be extended for bigger data set

Overall summary

Matrix

- Represent data in a matrix form with rows and columns representing samples and attributes respectively
- Represent coefficients in several equations in a matrix form

Rank

- Number of independent variables or samples

Nullity

- Identifies the number of linear relationships (if any)

Null Space

- Null space vectors provide the linear relationhips