Fundamentals of Artificial Intelligence

Principal Component Analysis

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Machine Learning

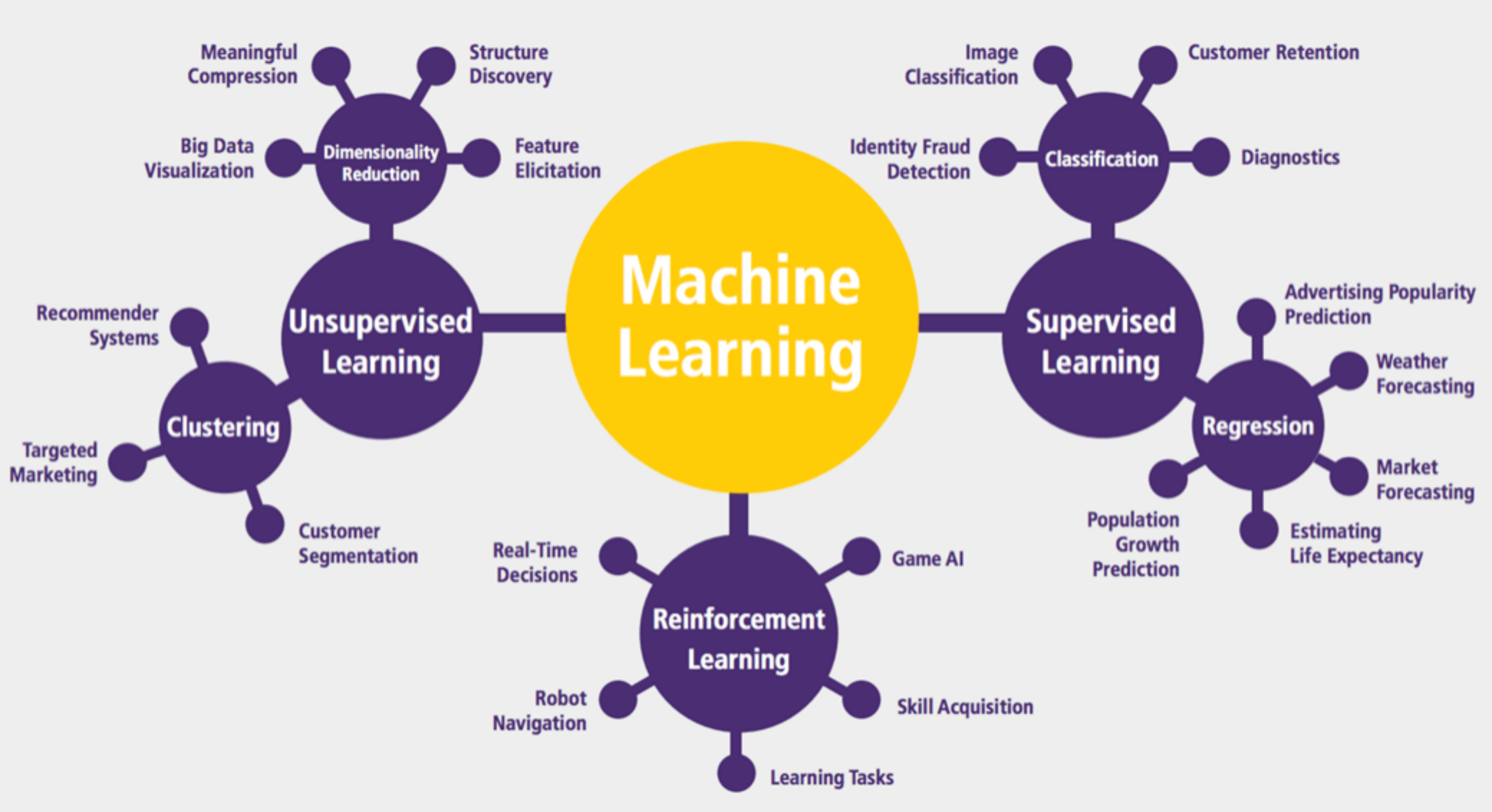


Image Source: DHL, Artificial Intelligence in Logistics, 2018.

Dimensionality Reduction

Dimensionality is the number of variables, characteristics or features present in the dataset. In most cases, the features are correlated and, therefore, there is some information that is redundant which increase the dataset's noise.

This redundant information impacts negatively in Machine Learning model's training and performance and that is why using dimensionality reduction methods becomes of paramount importance.

Dimensionality reduction is the process of reducing the number of random variables under consideration, by obtaining a set of principal variables.

Dimensionality Reduction

Categories:

Dimension reduction: to reduce the training complexity;
E.g., dataset representation, data pre-processing.

a. Feature selection: Find a subset of the original set of variables, or features, to get a smaller subset which can be used to model the problem.

b. Feature extraction: Reduces the data in a high dimensional space to a lower dimension space, i.e. a space with lesser no. of dimensions. The output features will not be the same as the originals.

When using feature extraction, we project the data into a new feature space, so the new features will be combinations of the original features, compressed in a way that they will retain the most relevant information.

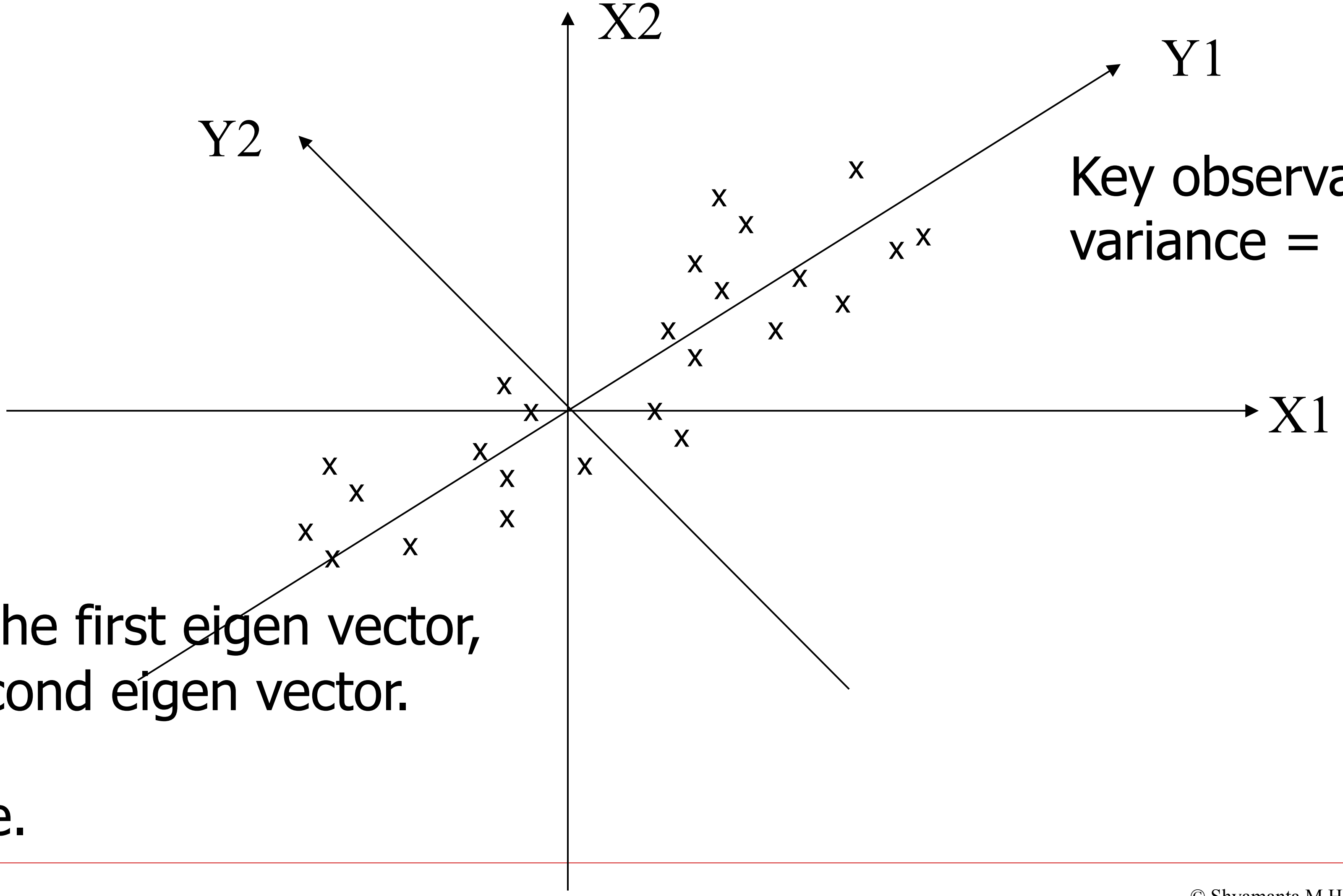
Principal Components Analysis

- An exploratory technique used to reduce the dimensionality of the data set.

> Exploratory Data Analysis (EDA) is a process of describing the data by means of statistical and visualization techniques in order to bring important aspects of that data into focus for further analysis. This involves inspecting the dataset from many angles, describing & summarizing it without making any assumptions about its contents.

- Can be used to:
  - Reduce number of dimensions in data
  - Find patterns in high-dimensional data
  - Visualize data of high dimensionality
- Example applications:
  - Face recognition
  - Image compression
  - Gene expression analysis

Principal Components Analysis



Key observation:
variance = largest!

Note: Y1 is the first eigen vector,
Y2 is the second eigen vector.

Y2 ignorable.

Principal Components Analysis

- Does the data set 'span' the whole of d dimensional space?
  - For a matrix of *n* samples x *n* instances, create a new covariance matrix of size *n* x *n*.
  - Transform some large number of variables into a smaller number of uncorrelated variables called principal components (PCs).
  - Developed to capture as much of the variation in data as possible!

Principal Components Analysis

Goal: Find r-dim projection that best preserves variance

1. Compute mean vector μ and covariance matrix Σ of original points

2. Compute eigenvectors and eigenvalues of Σ

3. Select top r eigenvectors

4. Project points onto subspace spanned by them:

$$y = A(x - \mu)$$

   where y is the new point, x is the old one, and the rows of A are the eigenvectors

Principal Components Analysis

- Question: how much spread is in the data along the axis? (distance to the mean)

- Variance=Standard deviation^2

$$s^2 = \frac{\sum_{i=1}^{n} (X_i - \bar{X})^2}{(n-1)}$$

Temperature
42
40
24
30
15
18
15
30
15
30
35
30

Principal Components Analysis

Covariance:
measures the correlation between X and Y

- cov(X,Y)=0: independent
- cov(X,Y)>0: move same dir
- cov(X,Y)<0: move oppo dir

$$\operatorname{cov}(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

X=Temperature	Y=Humidity
40	90
40	90
40	90
30	90
15	70
15	70
15	70
30	90
15	70
30	70
30	70
30	90

Principal Components Analysis

- Contains covariance values between all possible dimensions (attributes):

$$C^{nxn} = (c_{ij} \mid c_{ij} = \mathrm{cov}(Dim_i, Dim_j))$$

- Example for three attributes (x,y,z):

$$C = \begin{pmatrix} \mathrm{cov}(x,x) & \mathrm{cov}(x,y) & \mathrm{cov}(x,z) \\ \mathrm{cov}(y,x) & \mathrm{cov}(y,y) & \mathrm{cov}(y,z) \\ \mathrm{cov}(z,x) & \mathrm{cov}(z,y) & \mathrm{cov}(z,z) \end{pmatrix}$$

Eigenvalues and Eigenvectors

In linear algebra, it is often important to know which vectors have their directions unchanged by a given linear transformation. An **eigenvector** (/ˈaɪɡən-/ *EYE-gən-*) or **characteristic vector** is such a vector. Thus an eigenvector $\mathbf{v}$ of a linear transformation T is scaled by a constant factor λ when the linear transformation is applied to it: $T\mathbf{v} = \lambda\mathbf{v}$. The corresponding **eigenvalue**, **characteristic value**, or **characteristic root** is the multiplying factor λ.

- Vectors $\mathbf{x}$ having same direction as $A\mathbf{x}$ are called *eigenvectors* of A (A is an n by n matrix).

- In the equation $A\mathbf{x}=\lambda\mathbf{x}$, λ is called an *eigenvalue* of A.

Eigenvalues and Eigenvectors

- $A\mathbf{x}=\lambda\mathbf{x} \Leftrightarrow (A-\lambda \mathrm{I})\mathbf{x}=0$

- How to calculate **x** and λ:
  - Calculate $det(A-\lambda I)$, yields a polynomial (degree n)
  - Determine roots to $det(A-\lambda I)=0$, roots are eigenvalues λ
  - Solve $(A- \lambda I)\ \mathbf{x}=0$ for each λ to obtain eigenvectors **x**

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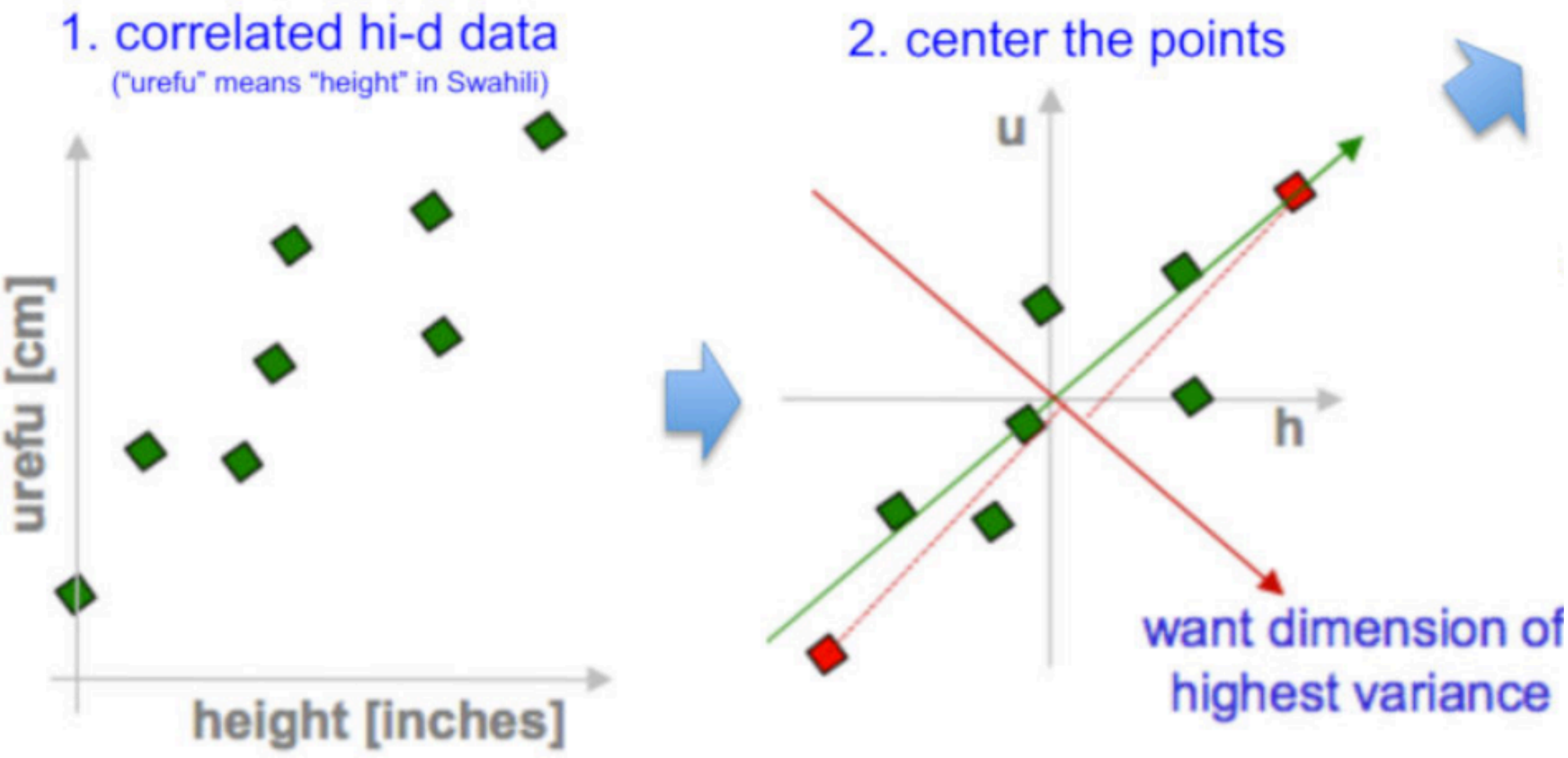
Eigenvalues and Eigenvectors

- 1st Principal Component (PC1)
  - The eigenvalue with the largest absolute value will indicate that the data have the largest variance along its eigenvector, the direction along which there is greatest variation
- 2nd Principal Component (PC2)
  - The direction with maximum variation left in data, orthogonal to the 1st PC
- In general, only few directions manage to capture most of the variability in the data.

Eigenvalues and Eigenvectors

- Let $\overline{X}$ be the mean vector (taking the mean of all rows)
- Adjust the original data by the mean
  $X' = X - \overline{X}$
- Compute the covariance matrix C of adjusted X
- Find the eigenvectors and eigenvalues of C.

Principal Components Analysis



Principal Components Analysis

3. compute covariance matrix

$$\begin{array}{ccc} & h & u \\ \begin{array}{c} h \\ u \end{array} & \multicolumn{2}{c}{\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}} \end{array} \qquad 0.8 \rightarrow \operatorname{cov}(h,u) = \frac{1}{n}\sum_{i=1}^{n} h_i u_i$$

4. eigenvectors + eigenvalues

$$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix} \begin{pmatrix} e_h \\ e_u \end{pmatrix} = \lambda_e \begin{pmatrix} e_h \\ e_u \end{pmatrix}$$

$$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix} \begin{pmatrix} f_h \\ f_u \end{pmatrix} = \lambda_f \begin{pmatrix} f_h \\ f_u \end{pmatrix}$$

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eig(cov(data))
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Principal Components Analysis