Northeastern University
College of Engineering

IE6600-Workshop

Visualizing with PCA

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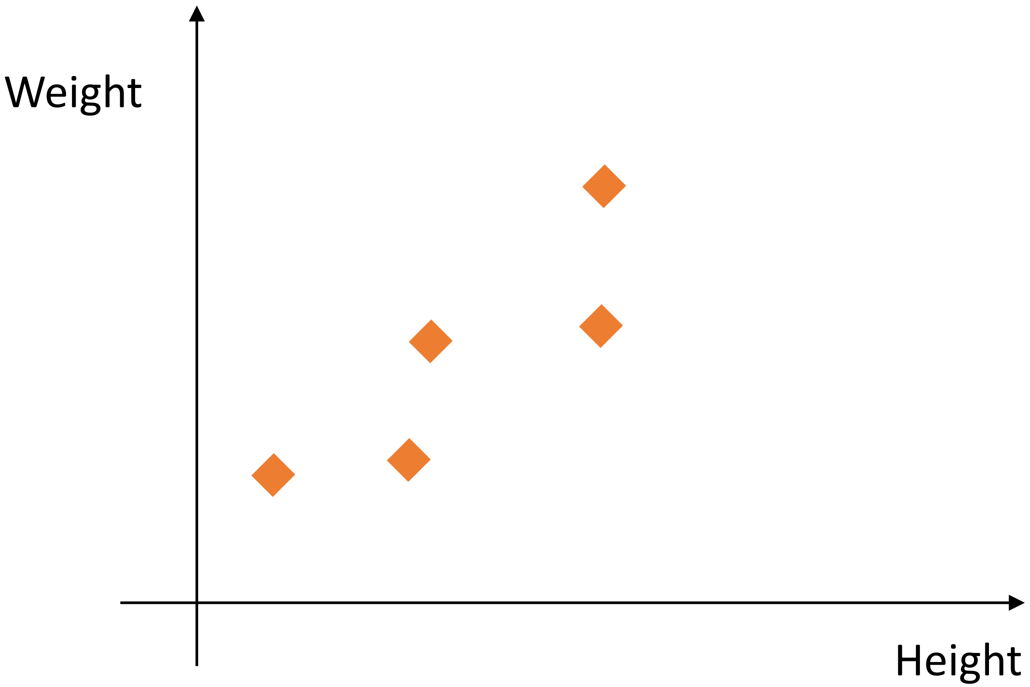
1. Curse of dimensionality

True vs. Observed Dimensionality

What is the dimensionality of this dataset?

ID	Observed Value (x_1) - Height (cm)	Predictive Value (y) – Weight (kg)
1	170	65
2	187	80
3	175	75
4	160	45
5	159	56



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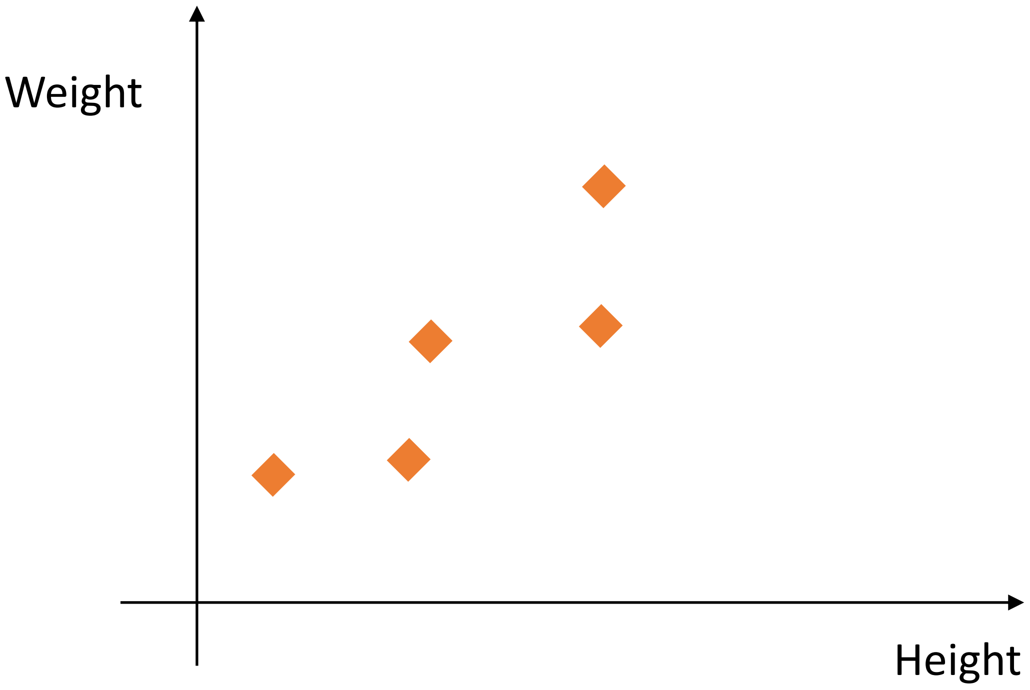
Observed Dimensionality: 6



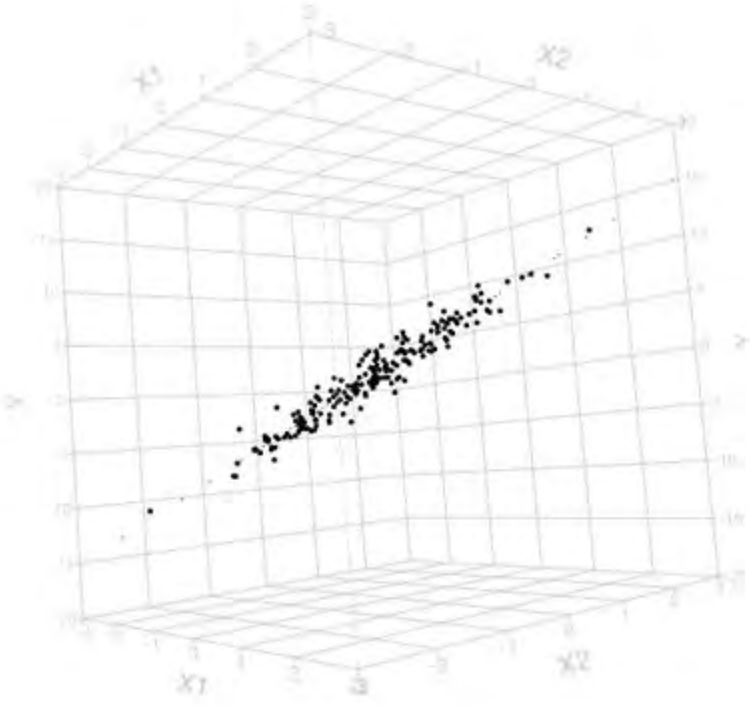
Features observed over time:

x_2: # of your waist (cm)
x_3: # of exams you have today
x_4: # of jokes you heard today
x_5: # of days left until summer

True vs. Observed Dimensionality

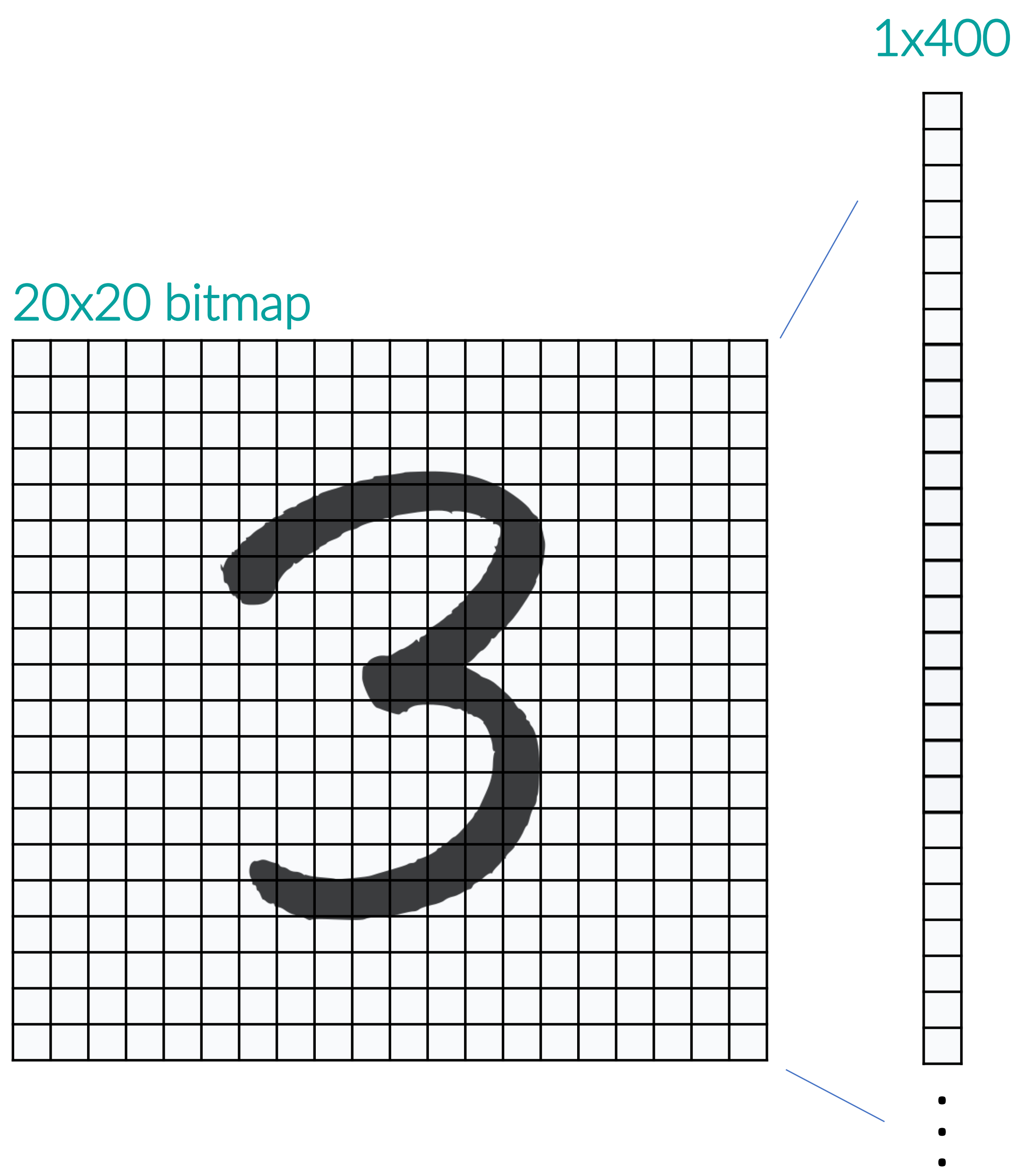
True Dimensionality: 3

ID	Observed Value (x_1) - Height (cm)	Observed value (x_2) - Waist (cm)	Predictive Value (y) – Weight (kg)
1	170	67	65
2	187	86	80
3	175	76	75
4	160	59	45
5	159	66	56



Curse of Dimensionality

Example:



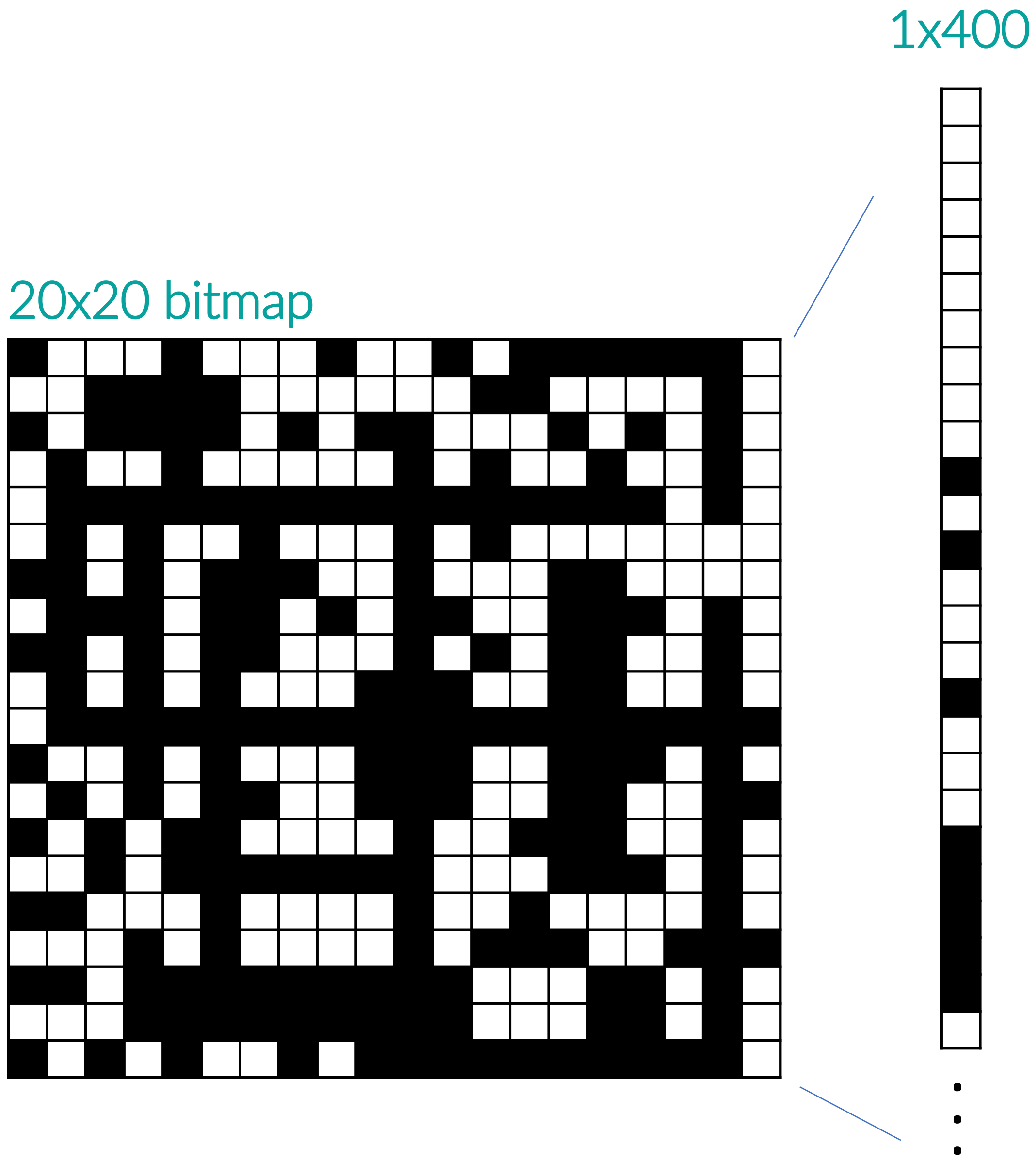
True Dimensionality

- 20x20 bitmap: $\{0, 1\}^{400}$ potential events
- The handwritten number THREE may be only 2^{40} events

Curse of Dimensionality

Example:

- 20x20 bitmap: $\{0, 1\}^{400}$ potential events
- Randomly sampling 2^{400} events



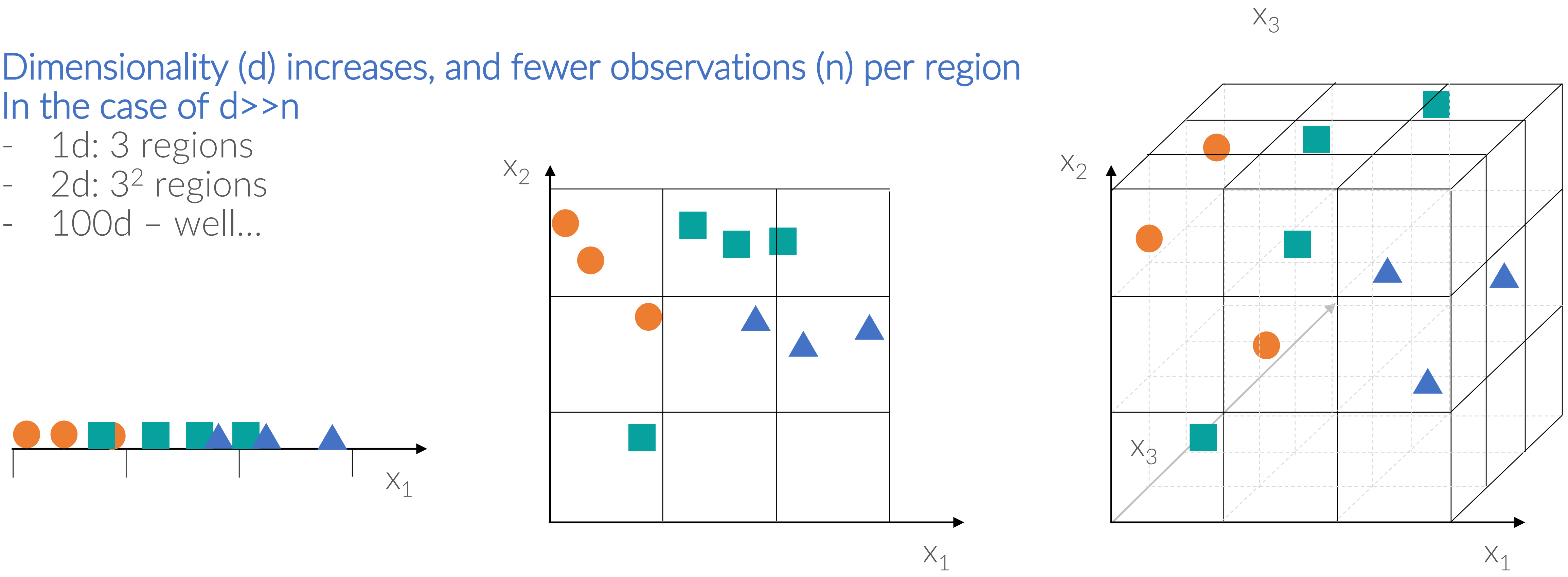
Curse of Dimensionality

Data mining/Machine learning methods are statistical

- Use numbers to build up the predictor f(x)
- Use categorical variables to classify: {0, 1}

Dimensionality (d) increases, and fewer observations (n) per region
In the case of d>>n

- 1d: 3 regions
- 2d: 3^2 regions
- 100d – well…



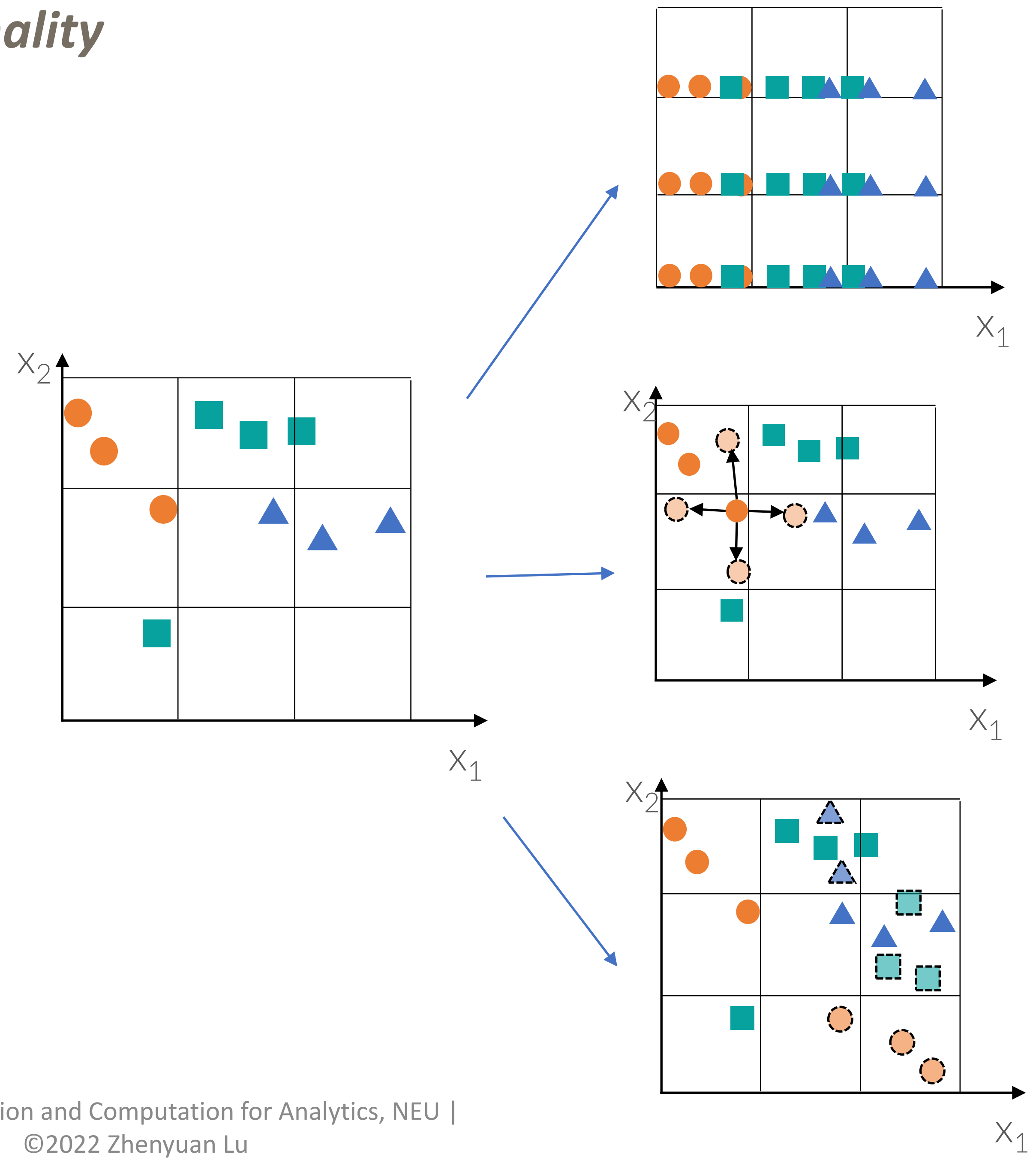
2.Methods of dealing with high dimensionality

Methods *Dealing with high dimensionality*

Use domain knowledge
- Feature engineering
- e.g. Testosterone -> Muscle building

Assumption on dimensions
- Independence: count along each dimension, e.g. Naïve bayes. When counting the frequency of x_1 ignore the x_2
- Smoothness: nearby region should have similar distribution of classes
- Symmetry: e.g. invariance to order of the dimensions: order doesn't matter

Reduce the dimensionality
- Create a new set of variables



Dimensionality Reduction

Feature selection

- Select a subset of the original dimension:

$$x_1, x_2, x_3, x_4\ x_5$$

- Discriminative: Select class as predictor

Feature extraction

- Construct a new set of dimensions:

$$E_i = f(x_1, x_2, x_3, x_4\ x_5)$$

$$E_1, E_2, E_3$$

$$x_1, x_2, x_3, x_4\ x_5$$

  - e.g. Linear combination of original dimensions: PCA

3.Principal components analysis (PCA)

One of the most beautiful ALGORITHMs

Principal Components Analysis (PCA)

The goal of PCA is to find a new set of dimensions (attributes) that better captures the variability of the data.

Some Math

Standard Basis Vector

d-dimensional Cartesian coordinate space is specified via the d unit vectors, called the standard basis vectors, along each of the axes. The j-th standard basis vector $\boldsymbol{e_j}$ is the d-dimensional unit vector whose j-th component is 1 and the rest of the components are 0

$$e_j = \left(0, 1_j, \dots, 0\right)^T$$

Any other vector in $\mathbb{R}^d$ can be written as linear combination of the standard basis vectors. For example, each of the points xi can be written as the linear combination

$$x_i = x_{i1}e_1 + x_{i2}e_2 + \cdots + x_{id}e_d = \sum_{j=1}^{d} x_{ij}e_j$$

where the scalar value x_{ij} is the coordinate value along the j-th axis or attribute

Standard Basis Vector

For example:

Consider the Iris data

	sepal length X_1	sepal width X_2	petal length X_3	petal width X_4	class X_5
$\mathbf{x}_1$	5.9	3.0	4.2	1.5	Iris-versicolor
$\mathbf{x}_2$	6.9	3.1	4.9	1.5	Iris-versicolor
$\mathbf{x}_3$	6.6	2.9	4.6	1.3	Iris-versicolor
$\mathbf{x}_4$	4.6	3.2	1.4	0.2	Iris-setosa
$\mathbf{x}_5$	6.0	2.2	4.0	1.0	Iris-versicolor
$\mathbf{x}_6$	4.7	3.2	1.3	0.2	Iris-setosa
$\mathbf{x}_7$	6.5	3.0	5.8	2.2	Iris-virginica
$\mathbf{x}_8$	5.8	2.7	5.1	1.9	Iris-virginica
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\mathbf{x}_{149}$	7.7	3.8	6.7	2.2	Iris-virginica
$\mathbf{x}_{150}$	5.1	3.4	1.5	0.2	Iris-setosa

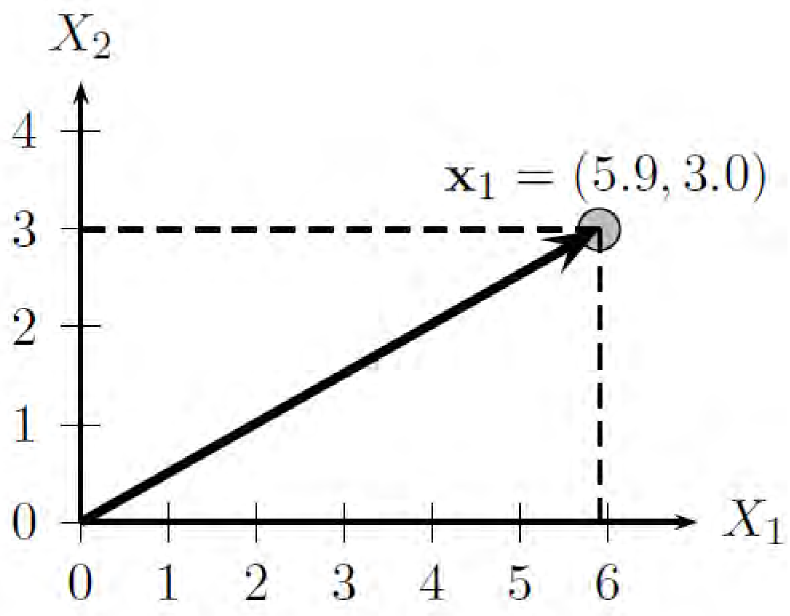
$$x_1 = (5.9, 3.0, 4.2)$$

$$x_1 = 5.9e_1 + 3.0e_2 + 4.2e_3 = 5.9\begin{pmatrix}1\\0\\0\end{pmatrix} + 3.0\begin{pmatrix}0\\1\\0\end{pmatrix} + 4.2\begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}5.9\\3.0\\4.2\end{pmatrix}$$

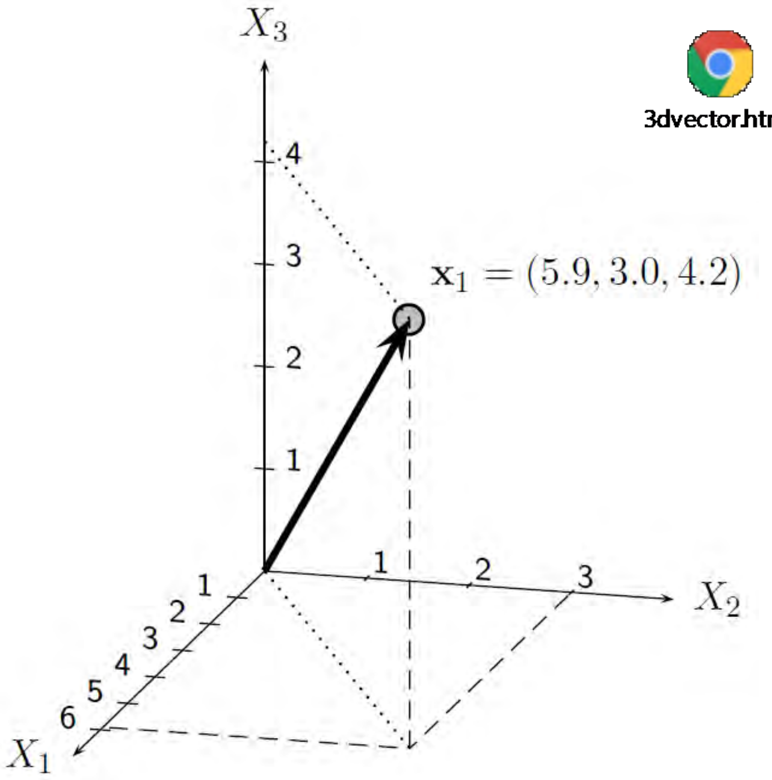
Geometric View

For example:

$$x_1 = (5.9, 3.0)$$
$$x_1 \in \mathbb{R}^2$$



$$x_1 = (5.9, 3.0, 4.2)$$
$$x_1 \in \mathbb{R}^3$$



3dvector.html

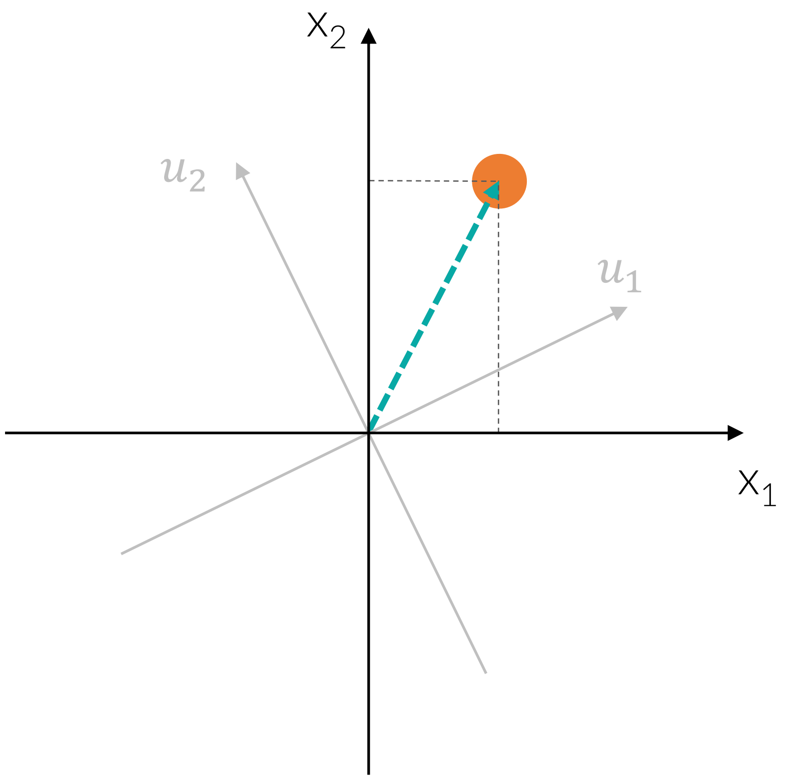
Original Points to New Coordinates

Let the data $\mathbf{D}$ consist of n points over d attributes, i.e., it is an $n \times d$ matrix, given as

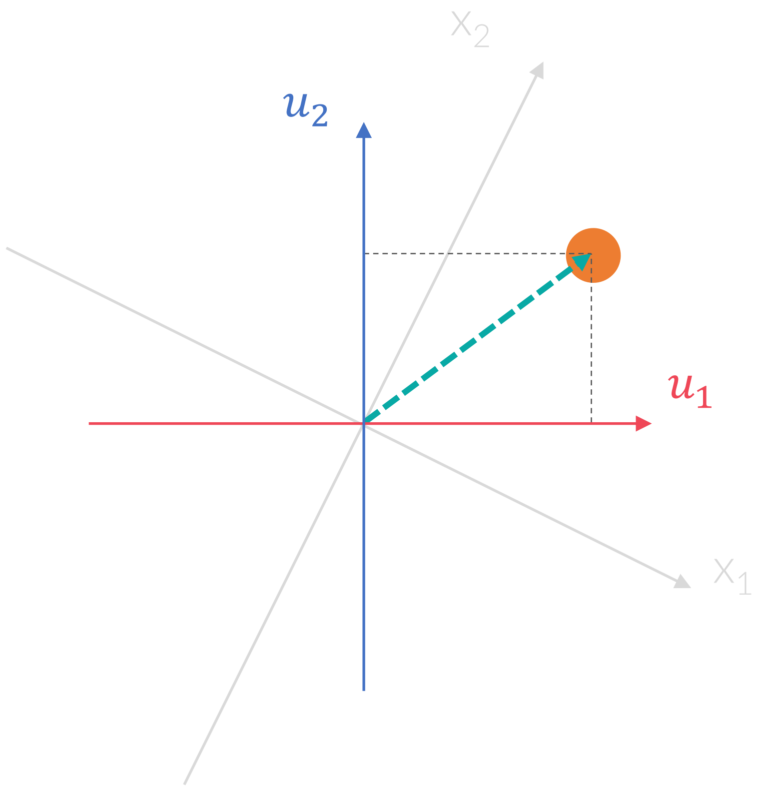
$$\mathbf{D} = \left(\begin{array}{c|cccc} & X_1 & X_2 & \cdots & X_d \\ \hline \mathbf{x}_1 & x_{11} & x_{12} & \cdots & x_{1d} \\ \mathbf{x}_2 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n & x_{n1} & x_{n2} & \cdots & x_{nd} \end{array}\right)$$

Each point $\mathbf{x}_i = (x_{i1}, x_{i2}, \cdots, x_{id})^T$ is a vector in the ambient d-dimensional vector space spanned by the d standard basis vectors $\mathbf{e}_1, \mathbf{e}_2, \cdots, \mathbf{e}_d$, where $\mathbf{e}_i$ corresponds to the i-th attribute X_i. Recall that the standard basis is an orthonormal basis for the data space, i.e., the basis vectors are pair-wise orthogonal, $\mathbf{e}_i^T \mathbf{e}_j = 0$, and have unit length $\|\mathbf{e}_i\| = 1$.

Original Points to New Coordinates



Original Basis



Optimal Basis

Original Points to New Coordinates

As such, given any other set of d orthonormal vectors $\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d$, with $\mathbf{u}_i^T \mathbf{u}_j = 0$ and $\|\mathbf{u}_i\| = 1$ (or $\mathbf{u}_i^T \mathbf{u}_i = 1$), we can re-express each point $\mathbf{x}$ as the linear combination

$$x = a_1 u_1 + a_2 u_2 + \cdots + a_d u_d$$

where the vector $\mathbf{a} = (a_1, a_2, \cdots, a_d)^T$ represents the coordinates of $\mathbf{x}$ in the new basis. The above linear combination can also be expressed as a matrix multiplication

$$x = Ua$$

where $\mathbf{U}$ is the $d \times d$ matrix, whose i-th column comprises the i-th basis vector $\mathbf{u}_i$

$$U = \begin{pmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_d \\ | & | & & | \end{pmatrix}$$

Original Points to New Coordinates

The matrix $\mathbf{U}$ is an *orthogonal* matrix, whose columns, the basis vectors, are *orthonormal*, i.e., they are pairwise orthogonal and have unit length

$$\mathbf{u}_i^T \mathbf{u}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Since $\mathbf{U}$ is orthogonal, this means that its inverse equals its transpose

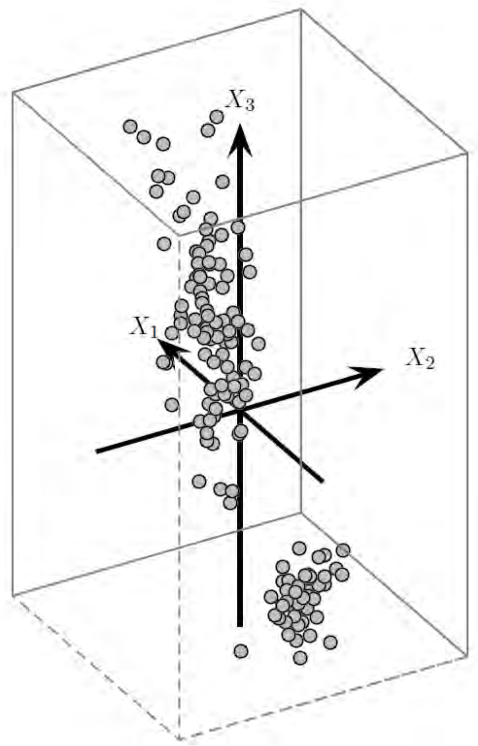
$$\mathbf{U}^{-1} = \mathbf{U}^T$$

which implies that $\mathbf{U}^T\mathbf{U} = \mathbf{I}$, where $\mathbf{I}$ is the $d \times d$ identity matrix.

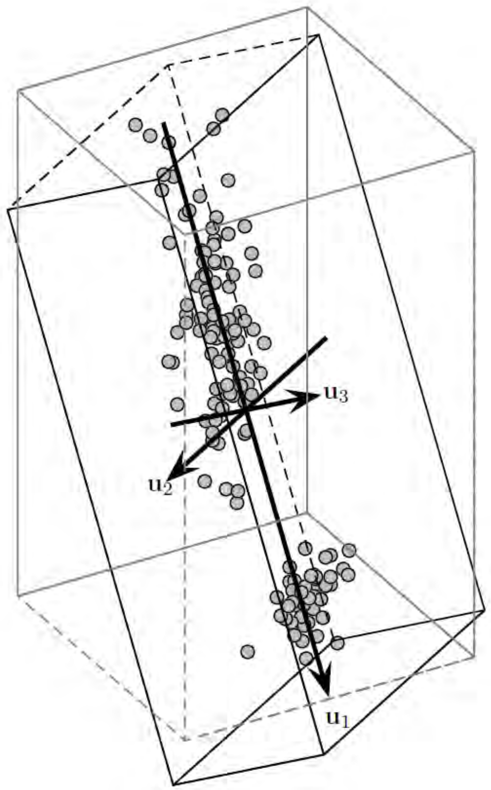
$$x = Ua$$
$$U^T x = U^T U a$$
$$a = U^T x$$

Original Points to New Coordinates

For example:



Original Basis



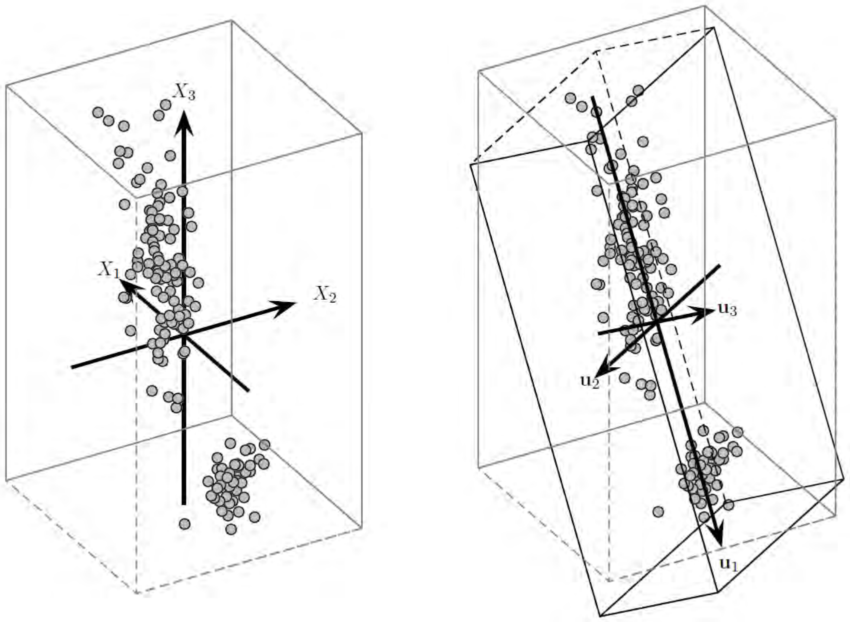
Optimal Basis

Mohammed J. Zaki, Wagner Meira, Jr., 2014

Original Points to New Coordinates

$$x = Ua$$
$$a = U^T x$$

For example:



$$u_1 = \begin{pmatrix} -0.390 \\ 0.089 \\ -0.916 \end{pmatrix} \quad u_2 = \begin{pmatrix} -0.639 \\ -0.742 \\ 0.200 \end{pmatrix} \quad u_3 = \begin{pmatrix} -0.663 \\ 0.664 \\ 0.346 \end{pmatrix}$$

The new coordinates of the centered point
$x = (-0.343, -0.754, 0.241)^T$ can be computed as:

$$a = U^T x = \begin{pmatrix} -0.390 & 0.089 & -0.916 \\ -0.639 & -0.742 & 0.200 \\ -0.663 & 0.664 & 0.346 \end{pmatrix} \begin{pmatrix} -0.390 \\ 0.089 \\ -0.916 \end{pmatrix} = \begin{pmatrix} -0.154 \\ 0.828 \\ -0.190 \end{pmatrix}$$

x can be written as the linear combination

$$x = -0.154u_1 + 0.828u_2 - 0.190u_3$$

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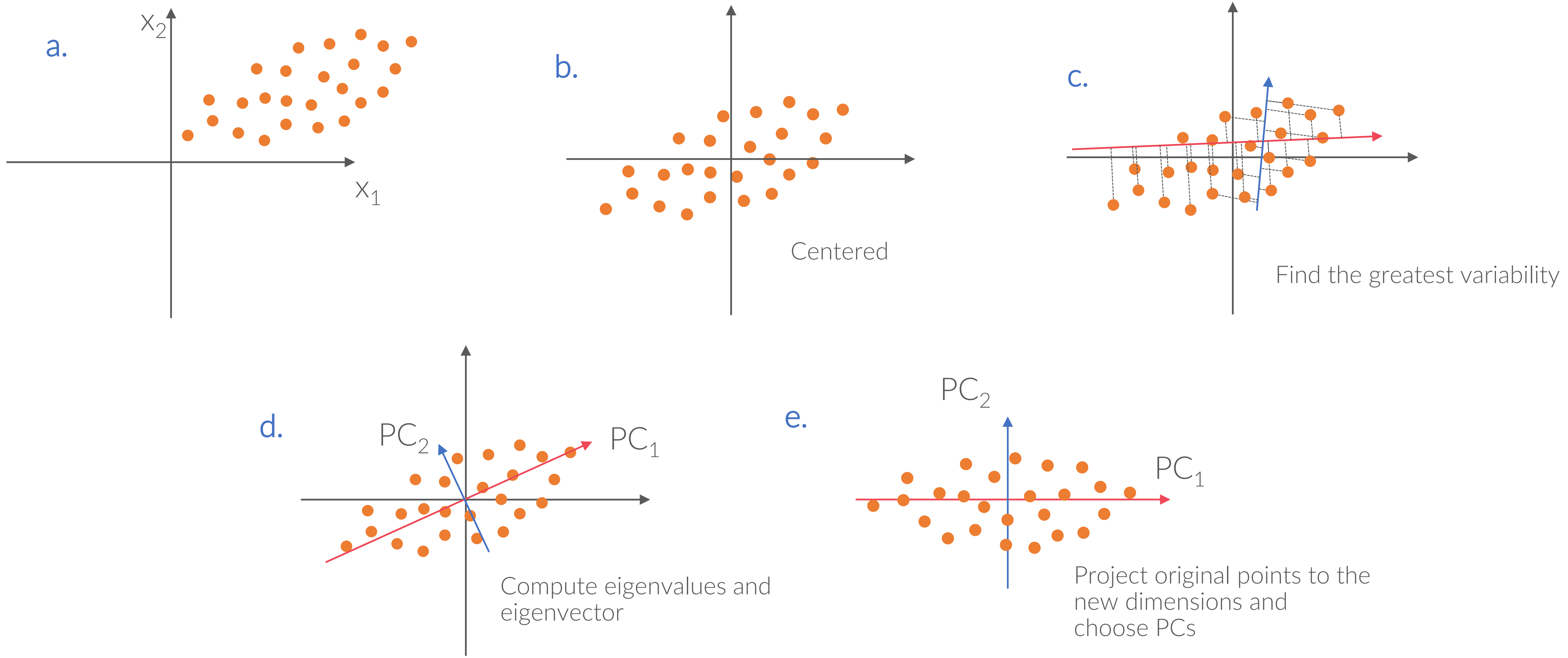
PCA

1. Find the first dimension to capture as much of the variability as possible
2. The second dimension is orthogonal to the first, and subject to that constraint, captures as much of the remaining variability.
3. And so on…until the d^{th} dimension.



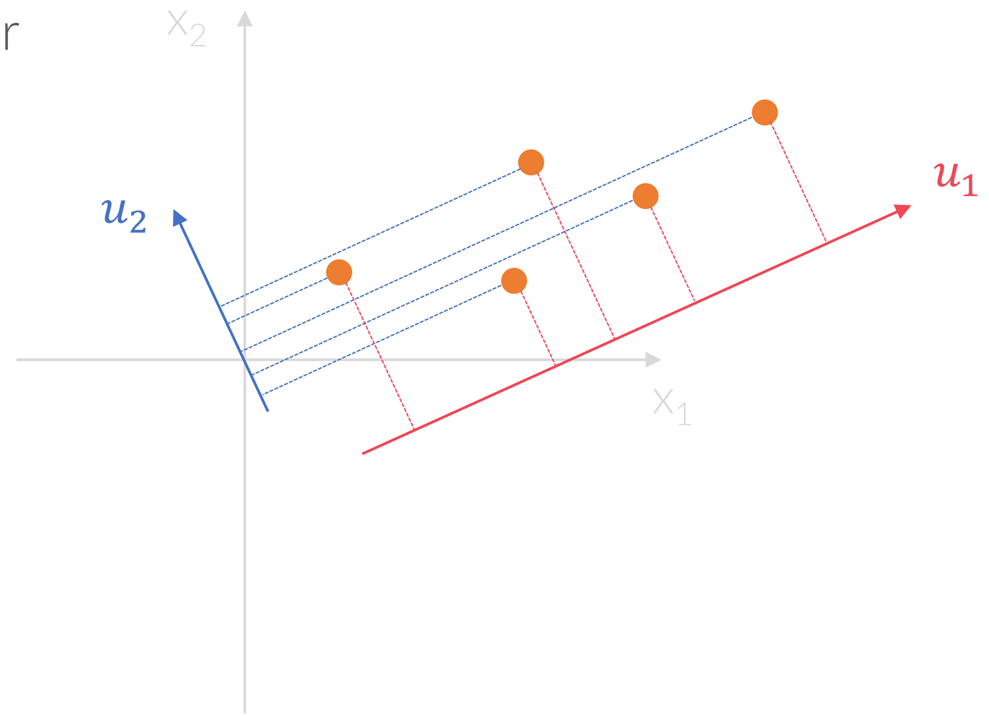
PCA *Why find greatest variability?*

Example:

We have a 2 dimensional data here to project all the data points to 1 dimension axis u_1, u_2 : {x_1, x_2} -> u_1, u_2

The data points in u_1-space are more expanded (greater variability) than in u_2-space.

1. Points are close in u_2-space but far in (x_1, x_2)-space which is not so ideal to represent the original dataset
2. The overall distances in u_1-space, with the highest variability, can represent the original distribution and variability



PCA *Find mean and center the data*

1. Center the data at zero: $Z = D - 1 \cdot \mu^T$

$$\mathbf{Z} = \mathbf{D} - \mathbf{1} \cdot \boldsymbol{\mu}^T = \begin{pmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_n^T \end{pmatrix} - \begin{pmatrix} \boldsymbol{\mu}^T \\ \boldsymbol{\mu}^T \\ \vdots \\ \boldsymbol{\mu}^T \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^T - \boldsymbol{\mu}^T \\ \mathbf{x}_2^T - \boldsymbol{\mu}^T \\ \vdots \\ \mathbf{x}_n^T - \boldsymbol{\mu}^T \end{pmatrix} = \begin{pmatrix} \mathbf{z}_1^T \\ \mathbf{z}_2^T \\ \vdots \\ \mathbf{z}_n^T \end{pmatrix}$$

Mohammed J. Zaki, Wagner Meira, Jr., Data Mining and Analysis: Fundamental Concepts and Algorithms, Cambridge University Press

PCA *Direction*

1. Center the data at zero: $Z = D - 1 \cdot \mu^T$
2. Covariance matrix $\Sigma = \frac{1}{n}(Z^T Z)$
   - covariance of x_1, x_2:
   - x_1, x_2 increase or decrease together or when one decreases the other one increases

Example

$cov(x_i, x_j) = \frac{(x_i-\mu_i)^T(x_j-\mu_j)}{n}$, After data centered: $\mu = 0$, $cov(x_i, x_j) = \frac{x_i^T x_j}{n}$

Say we have two sets of attributes $\sigma_1^2 = 2, \sigma_2^2 = 0.6$

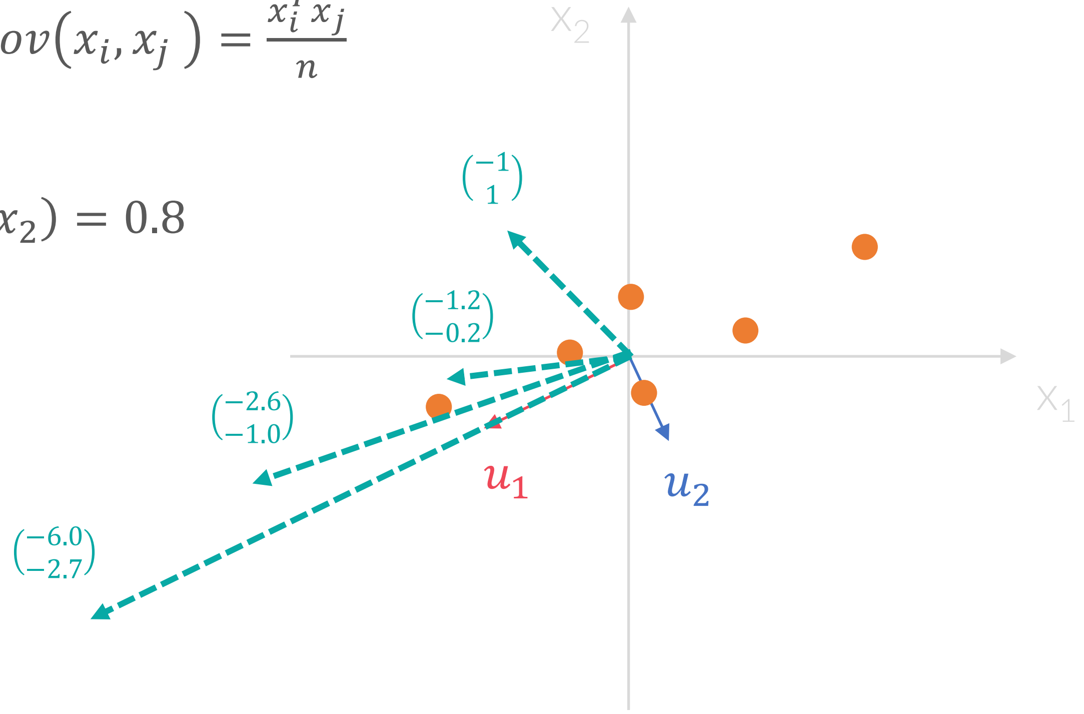
$$\begin{array}{ccc} & X_1 & X_2 \\ X_1 & \multicolumn{2}{c}{\multirow{2}{*}{$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}$}} \\ X_2 & & \end{array} \qquad cov(x_1, x_2) = 0.8$$

3. Multiply a vector $\begin{pmatrix} -1 \\ 1 \end{pmatrix}$ by $\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}$:

a. $\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1.2 \\ -0.2 \end{pmatrix}$ b. $\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} -1.2 \\ -0.2 \end{pmatrix} = \begin{pmatrix} -2.6 \\ -1.0 \end{pmatrix}$

c. $\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} -2.6 \\ -1.0 \end{pmatrix} = \begin{pmatrix} -6.0 \\ -2.7 \end{pmatrix} \rightarrow \begin{pmatrix} -14.1 \\ -6.4 \end{pmatrix} \rightarrow \begin{pmatrix} -33.3 \\ -15.1 \end{pmatrix}$

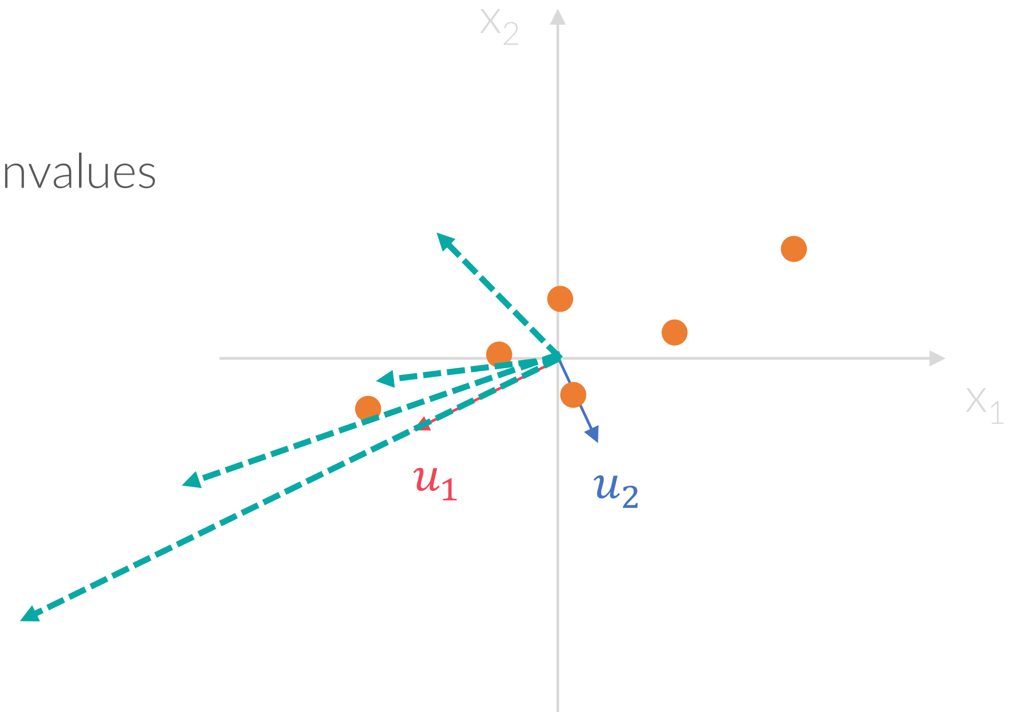
Slope: 0.45 0.454 0.454



Towards the greatest variance direction

PCA *Direction*

4. Look for a vector always keep in the same direction: $\sum u = \lambda u$
   - u : eigenvectors
   - $\sum$: covariance matrix
   - λ: scalar variable
   - Principal components = eigenvectors with largest eigenvalues



Towards the greatest variance direction

PCA *Find eigenvalues, eigenvector, and PCs*

1. Find eigenvalues by solving : $\sum \boldsymbol{u} = \boldsymbol{\lambda u} \rightarrow |\sum - \boldsymbol{\lambda I}| = \boldsymbol{0}$. $(\boldsymbol{NOTE}\text{: } \boldsymbol{Determinant\ of\ matrix\ A}: |\boldsymbol{A}|)$

- $\begin{vmatrix} 2.0-\lambda & 0.8 \\ 0.8 & 0.6-\lambda \end{vmatrix} = (2-\lambda)(0.6-\lambda) - 0.8 * 0.8 = \lambda^2 - 2.6\lambda + 0.56 = 0$
- $\{\lambda_1, \lambda_2\} = \frac{1}{2}\left(2.6 \pm \sqrt{2.6^2 - 4 * 0.56}\right) = \{2.36, 0.23\}$

2. Find $\boldsymbol{i^{th}}$ eigenvector by solving: $\sum \boldsymbol{u_i} = \boldsymbol{\lambda_i u_i}$

- $\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} u_{11} \\ u_{12} \end{pmatrix} = 2.36\begin{pmatrix} u_{11} \\ u_{12} \end{pmatrix}$

  $\rightarrow \begin{matrix} 2u_{11} + 0.8u_{12} = 2.36u_{11} \\ 0.8u_{11} + 0.6u_{12} = 2.36u_{12} \end{matrix} \rightarrow u_{11} = 2.2u_{12} \rightarrow u_1 \sim \begin{pmatrix} 2.2 \\ 1 \end{pmatrix},$

  $\rightarrow make\ ||u_1|| = 1, u_1 \frac{1}{\sqrt{2.2^2+1}}, then\ u_1 = \begin{pmatrix} 0.91 \\ 0.41 \end{pmatrix},$ slope = 0.454

- $\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} u_{21} \\ u_{22} \end{pmatrix} = 0.23\begin{pmatrix} u_{21} \\ u_{22} \end{pmatrix} \rightarrow then\ u_2 = \begin{pmatrix} -0.41 \\ 0.91 \end{pmatrix}$

3. $1^{st}\ PC$: $\begin{pmatrix} 0.91 \\ 0.41 \end{pmatrix}$, $2^{nd}\ PC$: $\begin{pmatrix} -0.41 \\ 0.91 \end{pmatrix}$

@ Victor Lavrenko

PCA *Fraction of total variance, and choose dimensionality*

Often we may not know how many dimensions, r, to use for a good approximation. One criteria for choosing r is to compute the fraction of the total variance captured by the first r principal components, computed as

$$f(r) = \frac{\lambda_1 + \lambda_2 + \cdots + \lambda_r}{\lambda_1 + \lambda_2 + \cdots + \lambda_d} = \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{d} \lambda_i} = \frac{\sum_{i=1}^{r} \lambda_i}{var(D)}$$

Given a certain desired variance threshold, say α, starting from the first principal component, we keep on adding additional components, and stop at the smallest value r, for which $f(r) \geq \alpha$ (α can be 0.9, 0.95 as purposes).

In practice, α is usually set to 0.9 or higher, so that the reduced dataset captures at least 90% of the total variance.

Algorithm 7.1: Principal Component Analysis

PCA $(\mathbf{D}, \alpha)$:

$\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$ `// compute mean`

$\mathbf{Z} = \mathbf{D} - \mathbf{1} \cdot \boldsymbol{\mu}^T$ `// center the data`

$\boldsymbol{\Sigma} = \frac{1}{n}\left(\mathbf{Z}^T\mathbf{Z}\right)$ `// compute covariance matrix`

$(\lambda_1, \lambda_2, \cdots, \lambda_d) = \text{eigenvalues}(\boldsymbol{\Sigma})$ `// compute eigenvalues`

$\mathbf{U} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_d \end{pmatrix} = \text{eigenvectors}(\boldsymbol{\Sigma})$ `// compute eigenvectors`

$f(r) = \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$, for all $r = 1, 2, \cdots, d$ `// fraction of total variance`

Choose smallest r so that $f(r) \geq \alpha$ `// choose dimensionality`

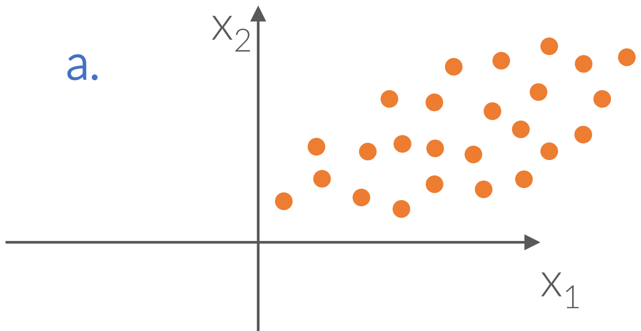
$\mathbf{U}_r = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_r \end{pmatrix}$ `// reduced basis`

$\mathbf{A} = \{\mathbf{a}_i \mid \mathbf{a}_i = \mathbf{U}_r^T \mathbf{x}_i, \text{for } i = 1, \cdots, n\}$ `// reduced dimensionality data`

Mohammed J. Zaki, Wagner Meira, Jr., Data Mining and Analysis: Fundamental Concepts and Algorithms

PCA

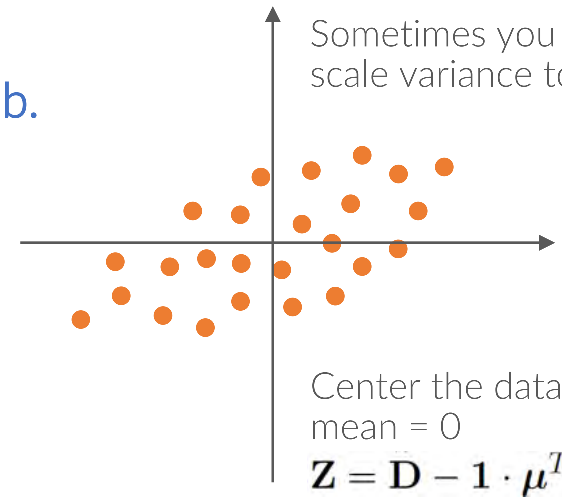
a.



Compute
the mean

$\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$

b.

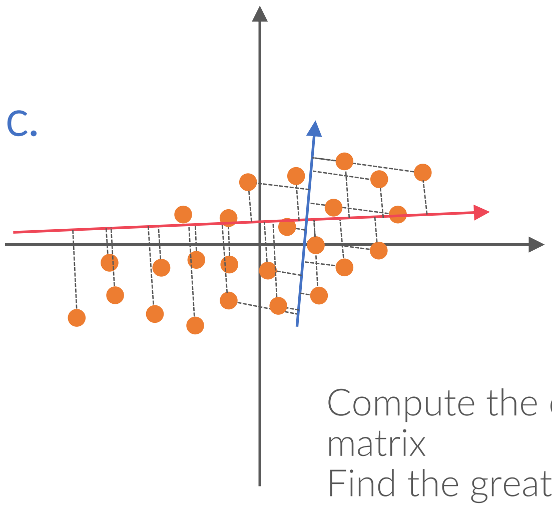


Sometimes you may also
scale variance to 1

Center the data, make
mean = 0

$\mathbf{Z} = \mathbf{D} - \mathbf{1} \cdot \boldsymbol{\mu}^T$

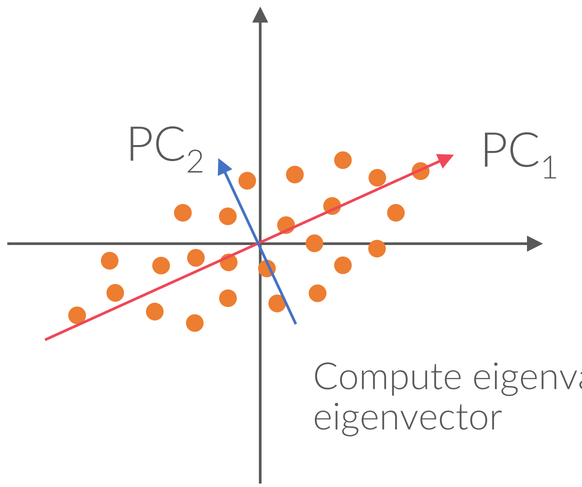
c.



Compute the covariance
matrix
Find the greatest variability

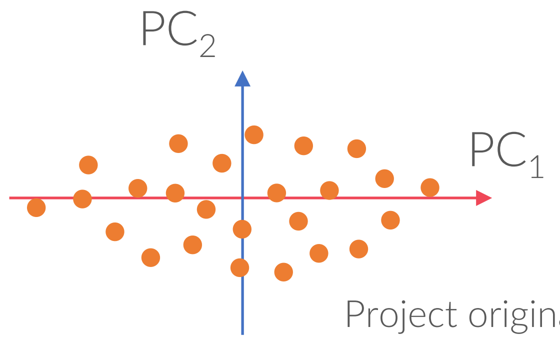
$\boldsymbol{\Sigma} = \frac{1}{n}\left(\mathbf{Z}^T\mathbf{Z}\right)$

d.



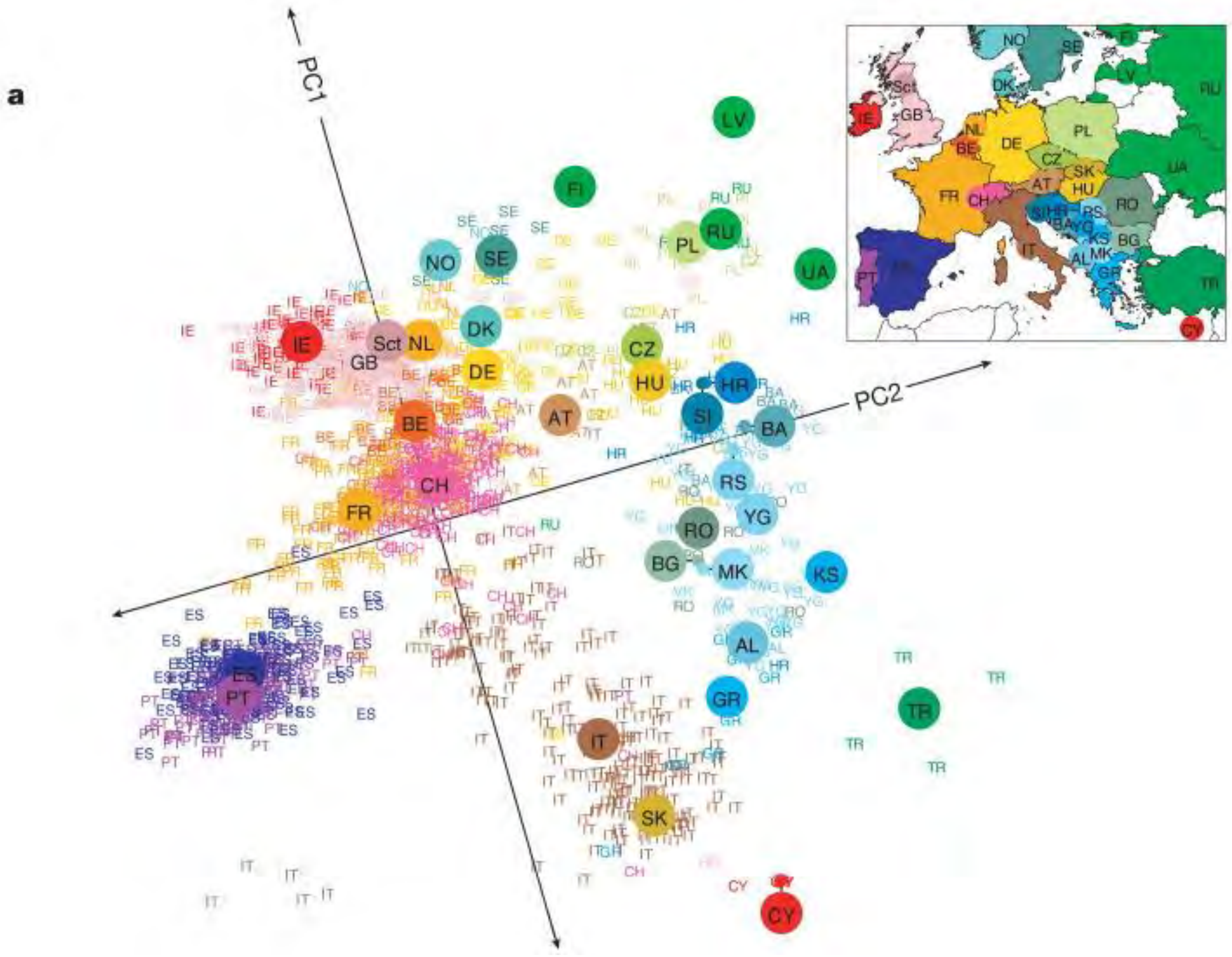
Compute eigenvalues and
eigenvector

e.



Project original points to the
new dimensions and
choose PCs

$f(r) = \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$



Novembre, John et al. "Genes mirror geography within Europe." Nature vol. 456,7218 (2008): 98-101. doi:10.1038/nature07331

Question

$$\sum = \begin{pmatrix} 0.681 & -0.039 & 1.265 \\ -0.039 & 0.187 & -0.320 \\ 1.265 & -0.32 & 3.092 \end{pmatrix}$$

$\lambda_1 = 3.662$ $\lambda_2 = 0.239$ $\lambda_3 = 0.059$

$u_1 = \begin{pmatrix} -0.39 \\ 0.089 \\ -0.916 \end{pmatrix}$ $u_2 = \begin{pmatrix} -0.639 \\ -0.742 \\ 0.200 \end{pmatrix}$ $u_3 = \begin{pmatrix} -0.663 \\ 0.664 \\ 0.346 \end{pmatrix}$

What is the total variance?
What is the fraction of total variance for each PC?
If let $\alpha = 0.95$ how many PCs we need to keep?

4.PCA Implementation in R

Algorithm 7.1: Principal Component Analysis

PCA $(\mathbf{D}, \alpha)$:

1. $\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$ `// compute mean`
2. $\mathbf{Z} = \mathbf{D} - \mathbf{1} \cdot \boldsymbol{\mu}^T$ `// center the data`
3. $\boldsymbol{\Sigma} = \frac{1}{n}(\mathbf{Z}^T\mathbf{Z})$ `// compute covariance matrix`
4. $(\lambda_1, \lambda_2, \cdots, \lambda_d) = \text{eigenvalues}(\boldsymbol{\Sigma})$ `// compute eigenvalues`
5. $\mathbf{U} = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_d) = \text{eigenvectors}(\boldsymbol{\Sigma})$ `// compute eigenvectors`
6. $f(r) = \frac{\sum_{i=1}^{r}\lambda_i}{\sum_{i=1}^{d}\lambda_i}$, for all $r = 1, 2, \cdots, d$ `// fraction of total variance`
7. Choose smallest r so that $f(r) \geq \alpha$ `// choose dimensionality`
8. $\mathbf{U}_r = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_r)$ `// reduced basis`
9. $\mathbf{A} = \{\mathbf{a}_i \mid \mathbf{a}_i = \mathbf{U}_r^T\mathbf{x}_i, \text{for } i = 1, \cdots, n\}$ `// reduced dimensionality data`

```r
data("iris")
head(iris)
```

```r
irisCent <- iris %>% transmute(sL=Sepal.Length-mean(Sepal.Length),
                               sW=Sepal.Width-mean(Sepal.Width),
                               pL=Petal.Length-mean(Petal.Length),
                               pW=Petal.Width-mean(Petal.Width))
```

```r
ic <- cov(irisCent)
```

```r
# use eigen() function to compute eigenvalues and eigenvectors
ieigen <- eigen(ic)
ie <- ieigen$values
iv <- ieigen$vectors
row.names(iv) <- names(iris %>% select(-Species))
colnames(iv) <- paste0(rep("PC",ncol(iv)),1:ncol(iv)) # or
sprintf("PC%d",1:4)
```

```r
# Fraction of the total variance
fr <- ie/sum(ie)
```

```r
# Choose number of dimensionality
threshold <- function(x, th) {
  sum <- 0
  seq <- 0
  for (i in 1:length(x)) {
    sum <-  sum + x[i]
    if (sum >= th) {
      seq <- i
      break
    }
  }
  return(seq)
}


threshold(x=fr, 0.95)
```

Algorithm 7.1: Principal Component Analysis

PCA $(\mathbf{D}, \alpha)$:

$\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$ `// compute mean`

$\mathbf{Z} = \mathbf{D} - \mathbf{1} \cdot \boldsymbol{\mu}^T$ `// center the data`

$\boldsymbol{\Sigma} = \frac{1}{n}\left(\mathbf{Z}^T\mathbf{Z}\right)$ `// compute covariance matrix`

$(\lambda_1, \lambda_2, \cdots, \lambda_d) = \text{eigenvalues}(\boldsymbol{\Sigma})$ `// compute eigenvalues`

$\mathbf{U} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_d \end{pmatrix} = \text{eigenvectors}(\boldsymbol{\Sigma})$ `// compute eigenvectors`

$f(r) = \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$, for all $r = 1, 2, \cdots, d$ `// fraction of total variance`

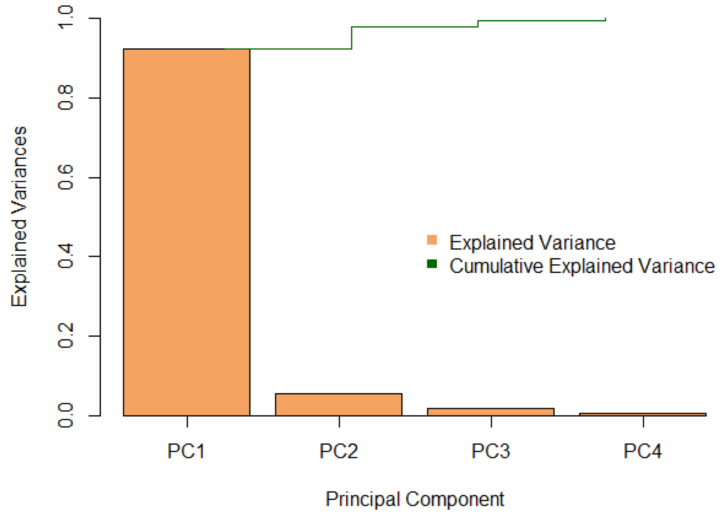
Choose smallest r so that $f(r) \geq \alpha$ `// choose dimensionality`

$\mathbf{U}_r = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_r \end{pmatrix}$ `// reduced basis`

$\mathbf{A} = \{\mathbf{a}_i \mid \mathbf{a}_i = \mathbf{U}_r^T \mathbf{x}_i, \text{for } i = 1, \cdots, n\}$ `// reduced dimensionality data`

```r
biPCA <- prcomp(iris[1:4], scale = TRUE)
biPCA$sdev^2/sum(biPCA$sdev^2)
biPCA$rotation
```

```r
barplot(
  fr,
  ylim = c(0, 1),
  col = "sandybrown",
  xlab = "Principal Component",
  ylab = "Explained Variances",
  axes = TRUE
)
axis(1, c(0.7, 1.9, 3.1, 4.3),
     labels = sprintf("PC%d", 1:4))
lines(cumsum(fr), type = 's', col = "darkgreen")
legend(
  x = 2.5,
  y = 0.5,
  legend = c("Explained Variance", "Cumulative
Explained Variance"),
  pch = c(15, 15),
  col = c("sandybrown", "darkgreen"),
  bty = 'n'
)
```



Algorithm 7.1: Principal Component Analysis

PCA $(\mathbf{D}, \alpha)$:

$\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$ `// compute mean`

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$f(r) = \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$, for all $r = 1, 2, \cdots, d$ `// fraction of total variance`

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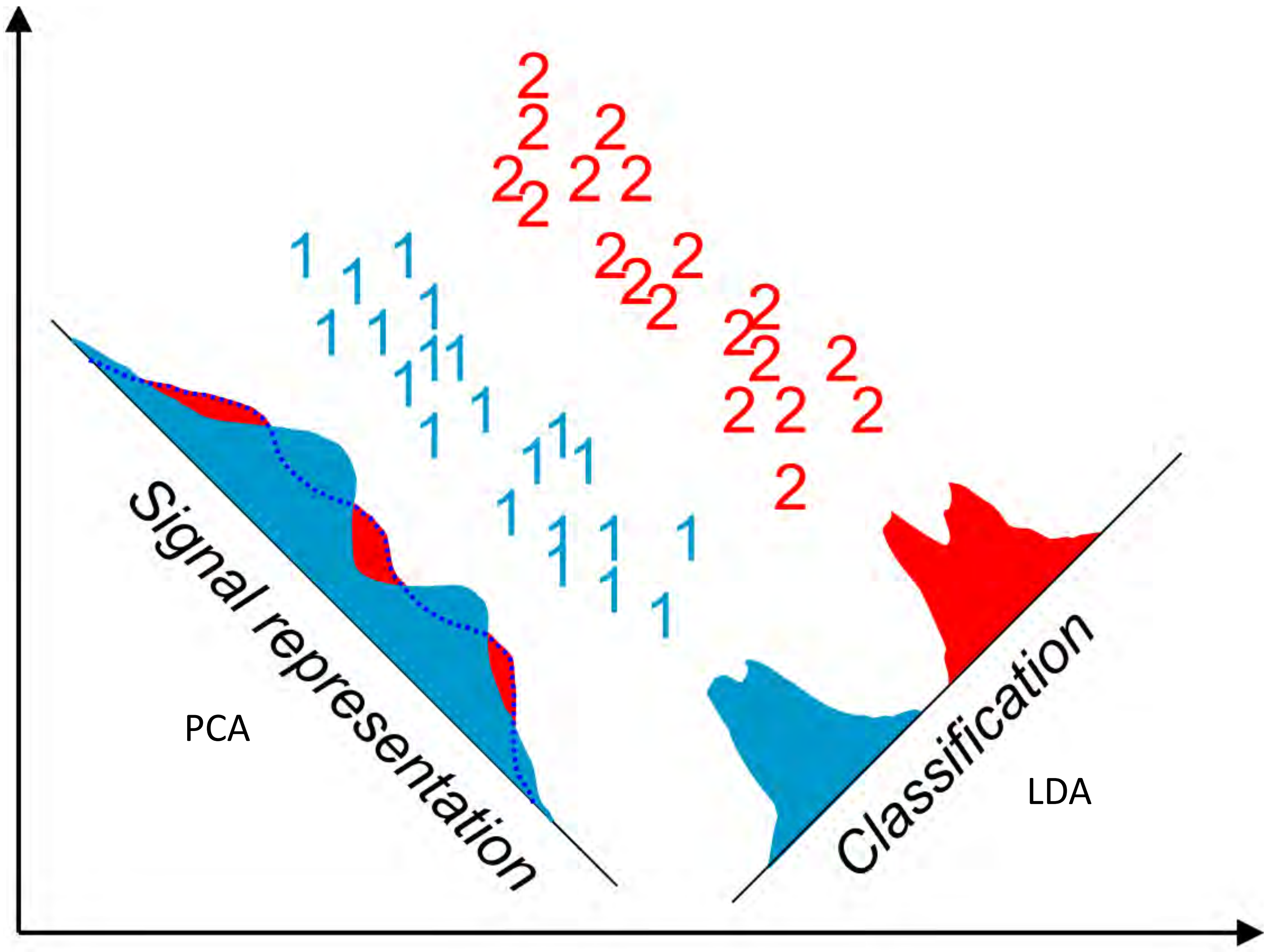
$\mathbf{U}_r = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_r \end{pmatrix}$ `// reduced basis`

$\mathbf{A} = \{\mathbf{a}_i \mid \mathbf{a}_i = \mathbf{U}_r^T \mathbf{x}_i, \text{for } i = 1, \cdots, n\}$ `// reduced dimensionality data`

Exercise:

1. Try three datasets: mpg, BostonHousing (mlbench), BreastCancer (mlbench) on two scale methods: a) mean=0, b)mean=0, variance=1.
2. Compare to the built-in PCA function prcomp()

PCA VS Linear Discriminant Analysis


Signal representation
PCA
Classification
LDA

5.PCA: Pros and Cons

PCA *Pros and Cons*

Pros

1. Good performance on processing speed
2. Reflects intuition on the data
3. Efficient reduction in size of data

Cons

1. Doesn’t consider class separability since it doesn’t take into account the class labels
2. PCA simply performs a coordinate rotation that aligns the transformed axes with the directions of maximum variance
3. There is no guarantee that the directions of maximum variance will contain good features for discrimination

   - PCA cannot recognize the class lables

Resources

Resource

Textbook:

Galit Shmueli, Peter C. Bruce, Inbal Yahav, Nitin R. Patel, Kenneth C. Lichtendahl Jr., Data Mining for Business Analytics: Concepts, Techniques, and Applications in R (DMBA), Wiley, 1st Edition, ISBN-10: 1118879368, ISBN-13: 978-1118879368.

Additional Textbooks:

R For Data Science (open license, R4DS), Wickham, Hadley, and Garrett Grolemund

R Markdown (open license, RMD), Xie, Yihui, et al.

James, Gareth, et al. An Introduction to Statistical Learning: with Applications in R. Springer, 2017. (open license, ISL)

Mohammed J. Zaki, Wagner Meira, Jr., Data Mining and Analysis: Fundamental Concepts and Algorithms, Cambridge University Press, May 2014. ISBN: 9780521766333.

David Hand, Heikki Mannila, Padhraic Smyth. Principles of Data Mining, The MIT Press, 2001, ISBN-10: 026208290X, ISBN-13: 978-0262082907.

Tan, Pang-Ning, et al. Introduction to Data Mining (DM). Pearson Education, 2006.

Materials

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