Machine Learning

Unsupervised Learning

Topics of previous lectures

- ✓ Ingredients of Machine Learning
- ✓ Classification Basics, Basic Linear Classifier
- ✓ K-Nearest Neighbours and Naive Bayes Classifier
- ✓ Linear and Quadratic Discriminant Analysis
- ✓ Support Vector Machines (SVM)
- ✓ Decision Trees
- ✓ Ensemble Methods (Bagging, Weighted Voting, Stacking)
- ✓ Regression Methods
- ✓ Evaluation and Scoring of Classifiers
- ✓ Ensemble Methods (Boosting)
- ✓ Clustering (Hierarchical, K-Means, K-Medoids, DBSCAN)

Topics of today's lecture

- Dimensionality Reduction
- Principal Component Analysis (PCA)
- t-Distributed Stochastic Neighbor Embedding (t-SNE)

Motivation for Dimensionality Reduction

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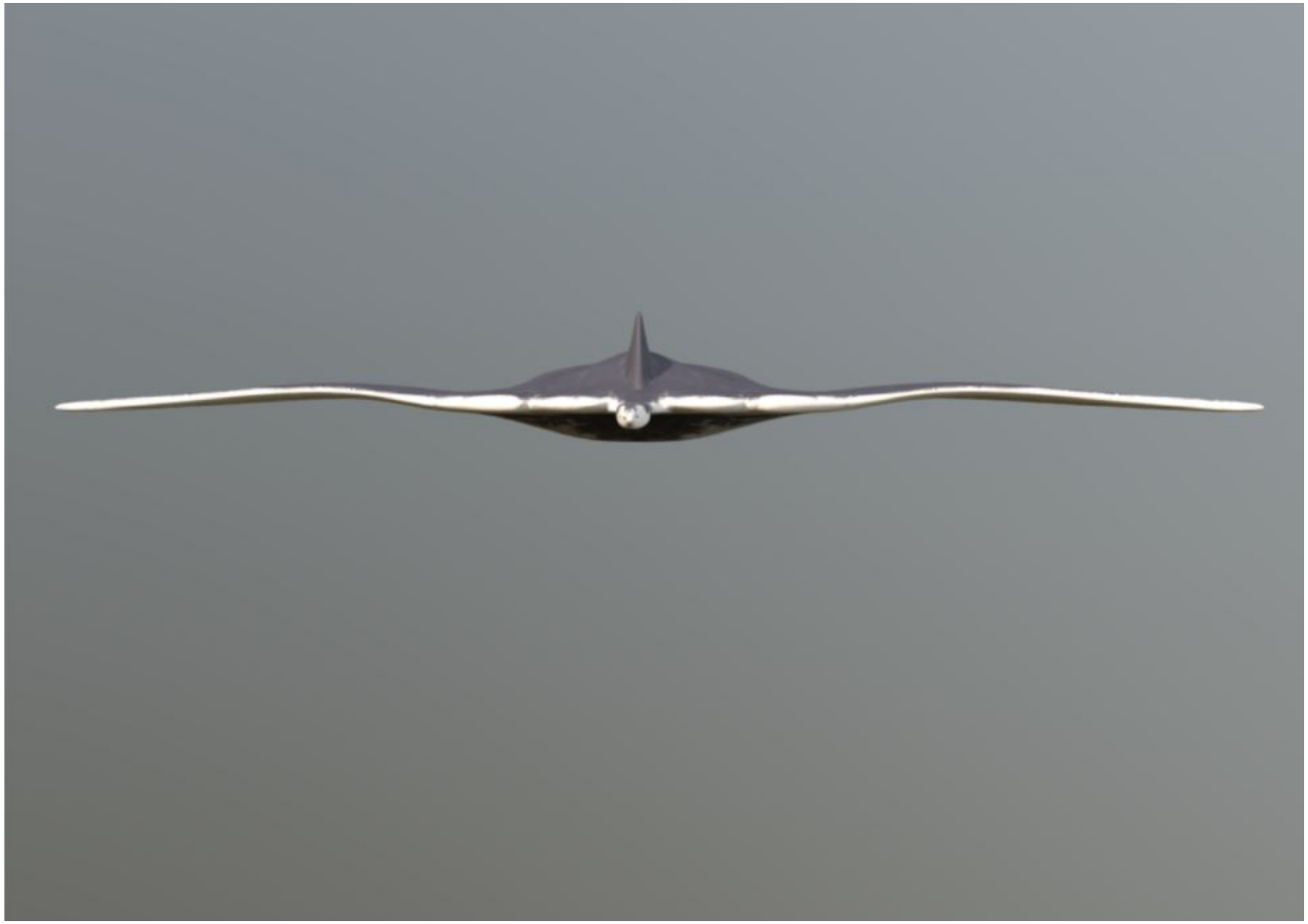
- It can also be useful to detect potential patterns in high dimensial data, by visualizing the first 2-3 projections.

Motivation for Dimensionality Reduction



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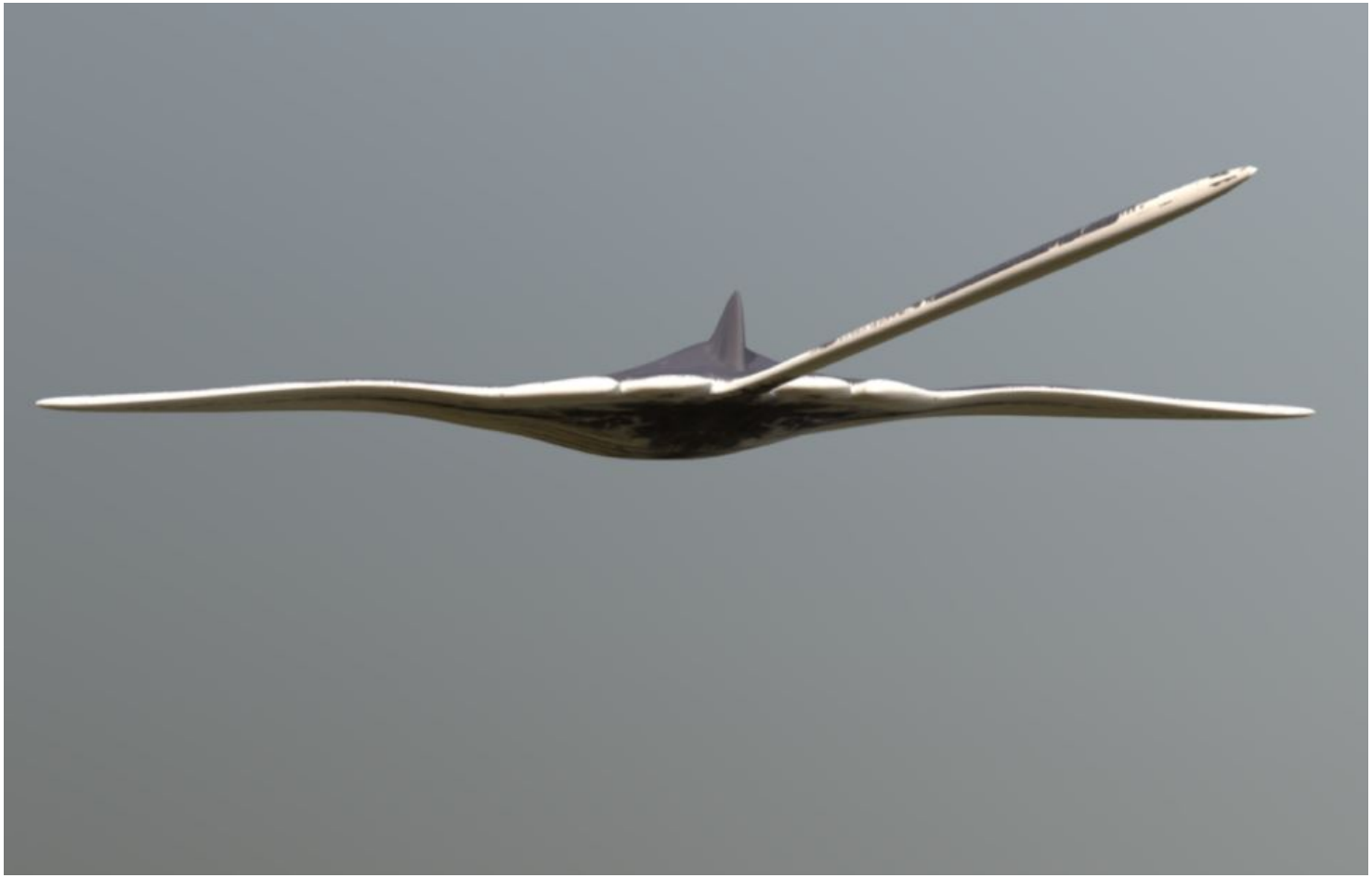

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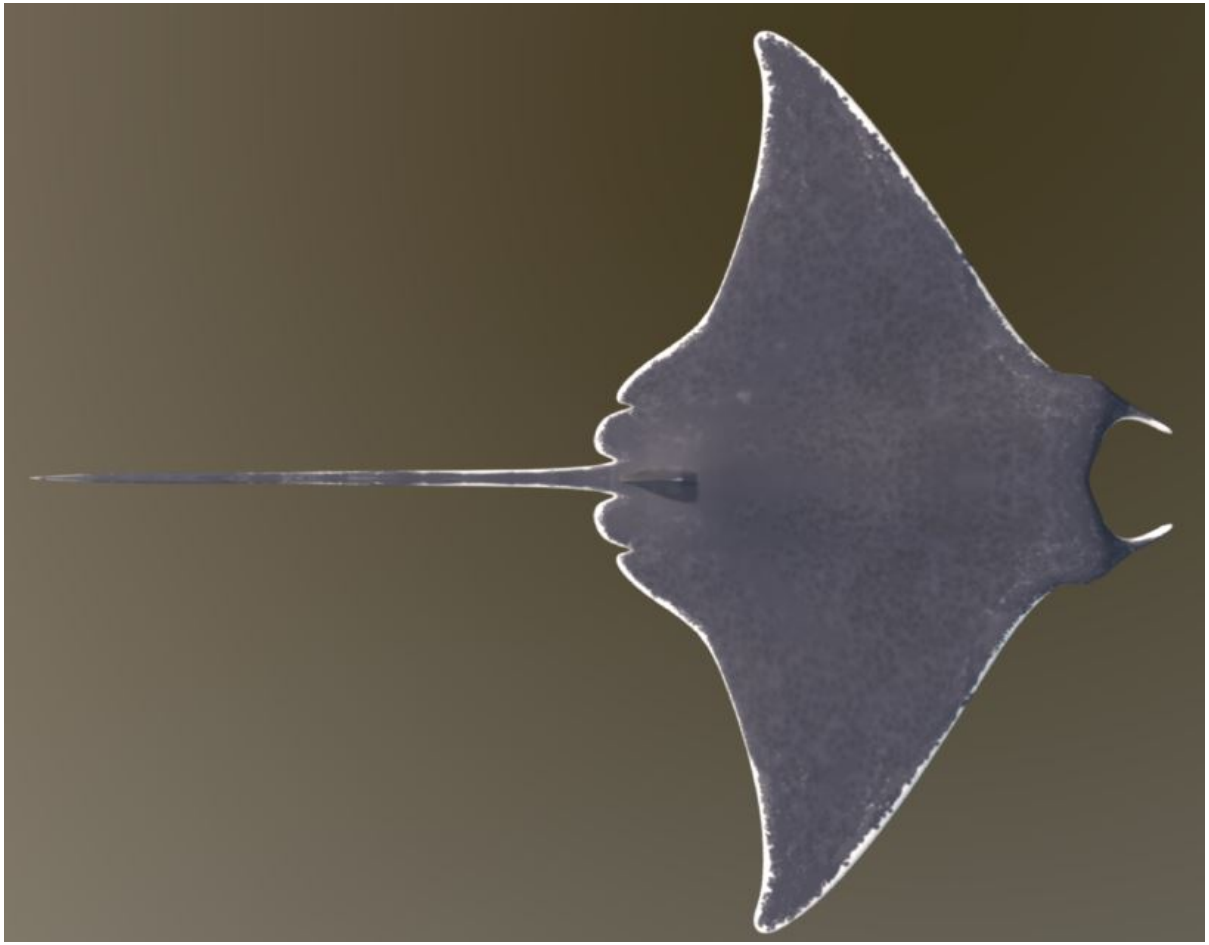
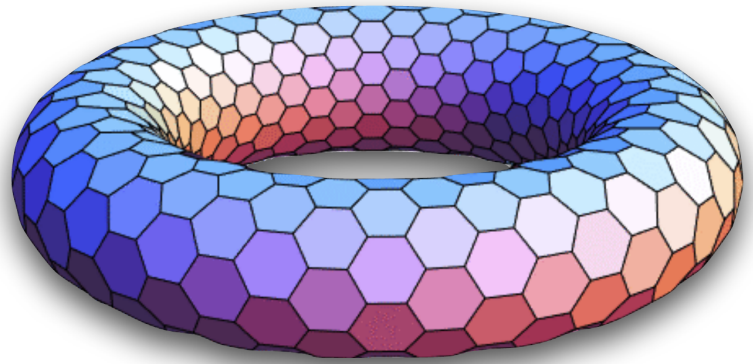


Principal Component Analysis

What is the problem with **high-dimensional** things?



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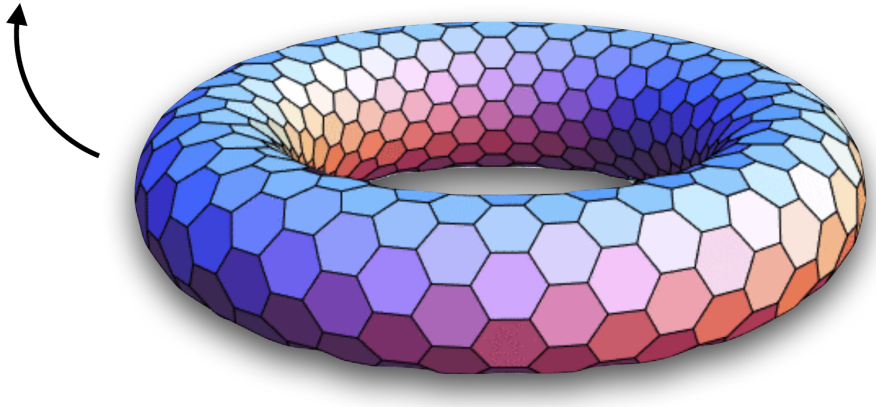

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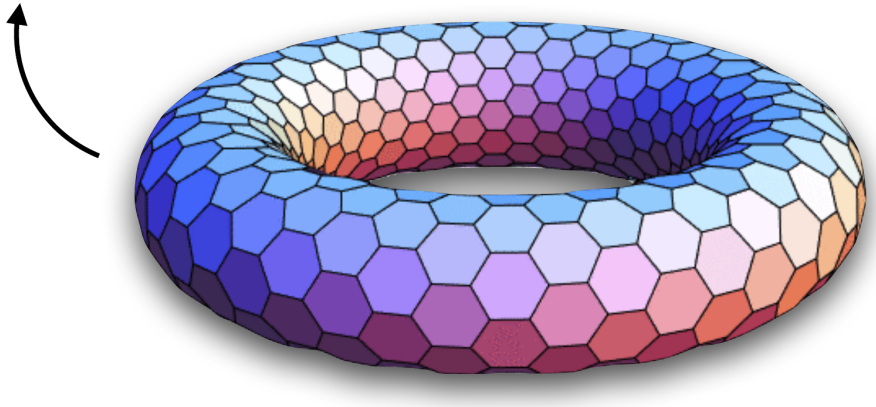

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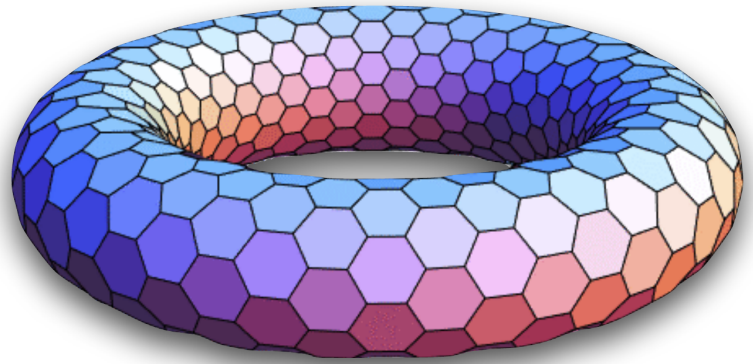

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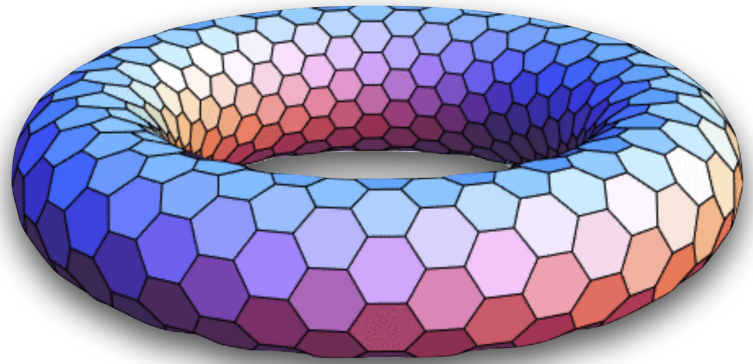

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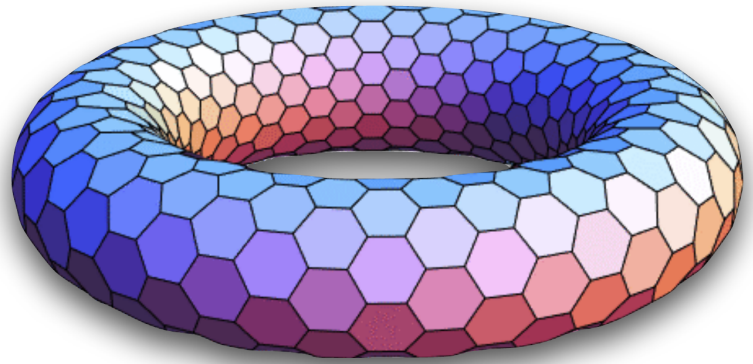

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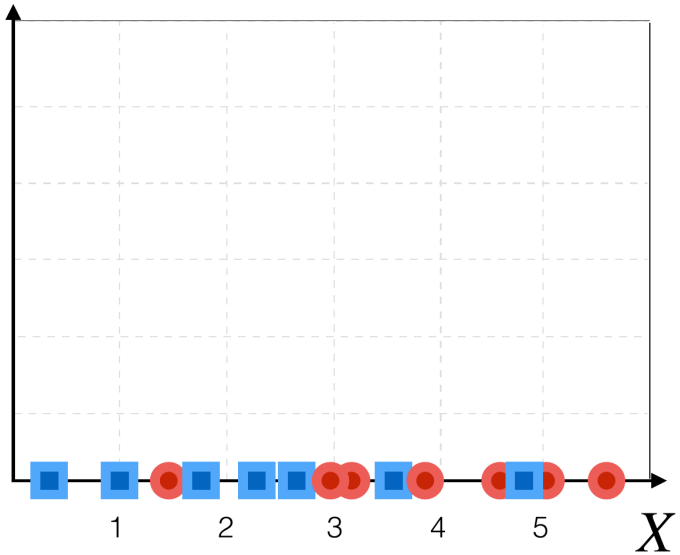

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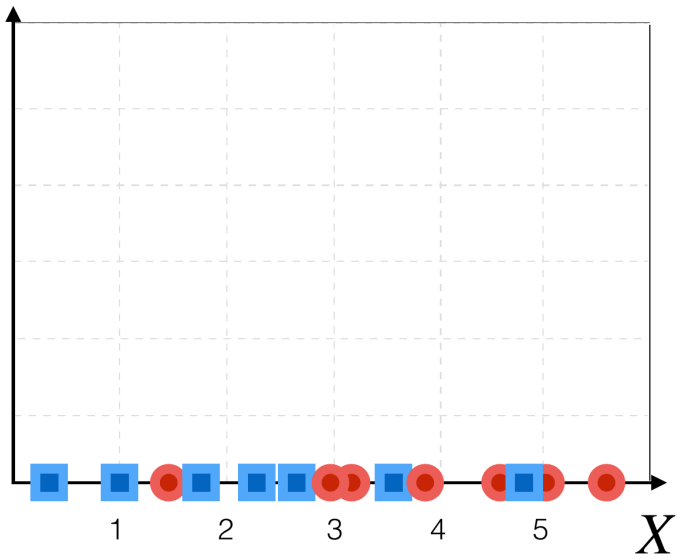

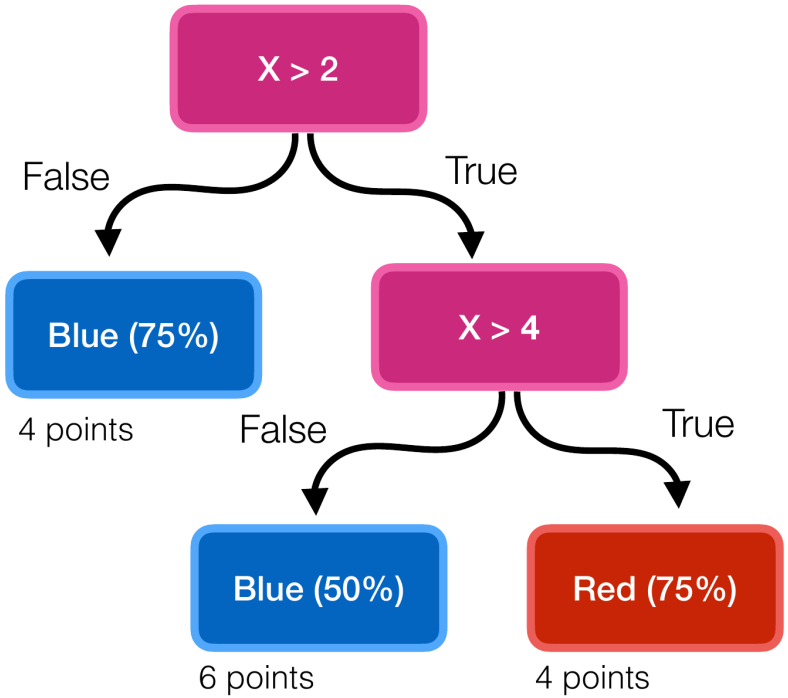

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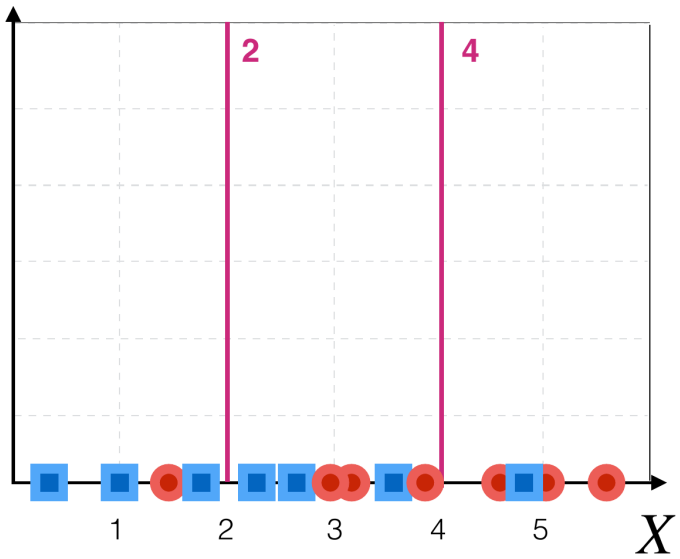

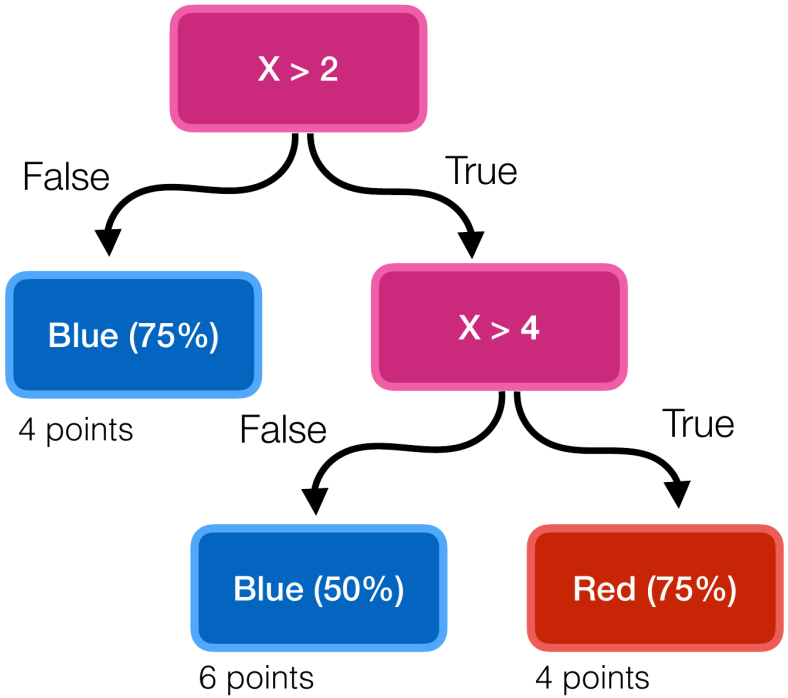

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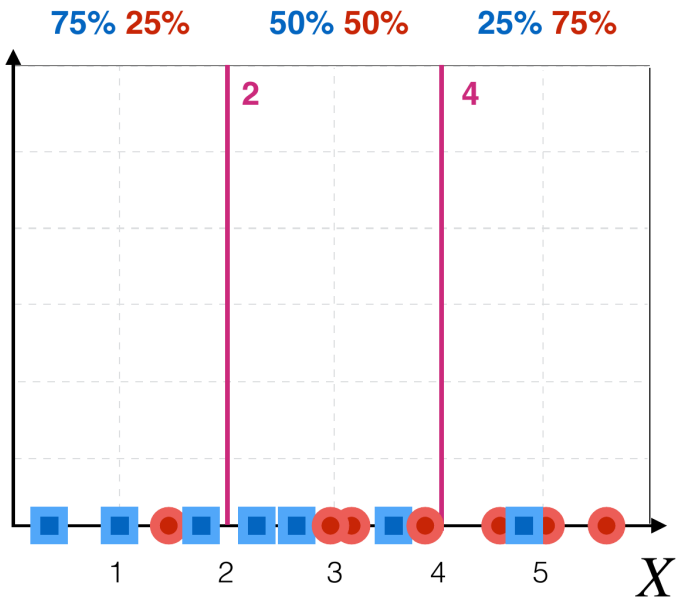

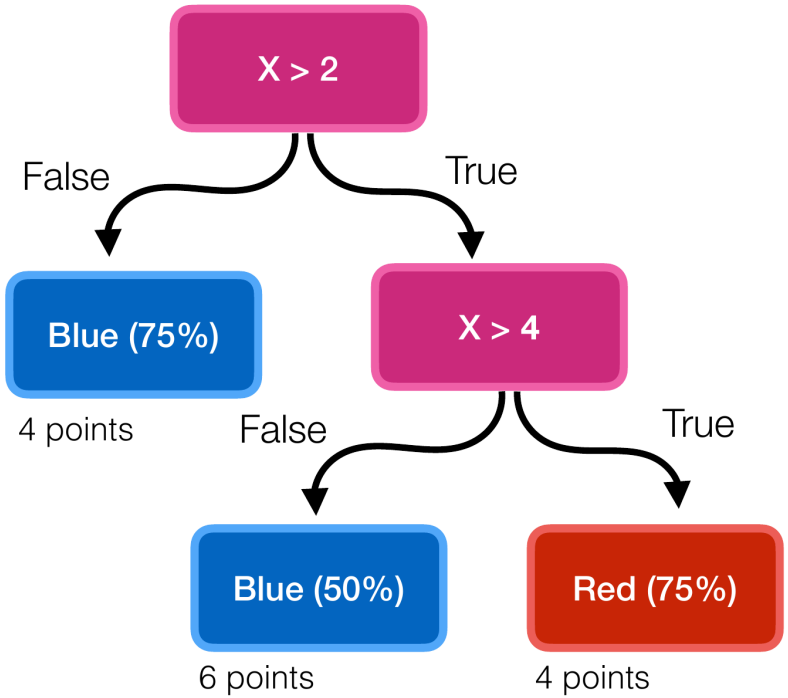

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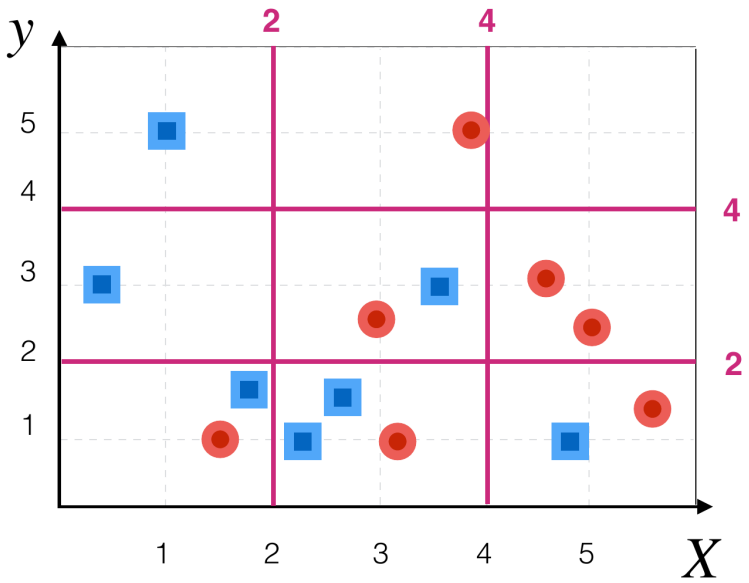

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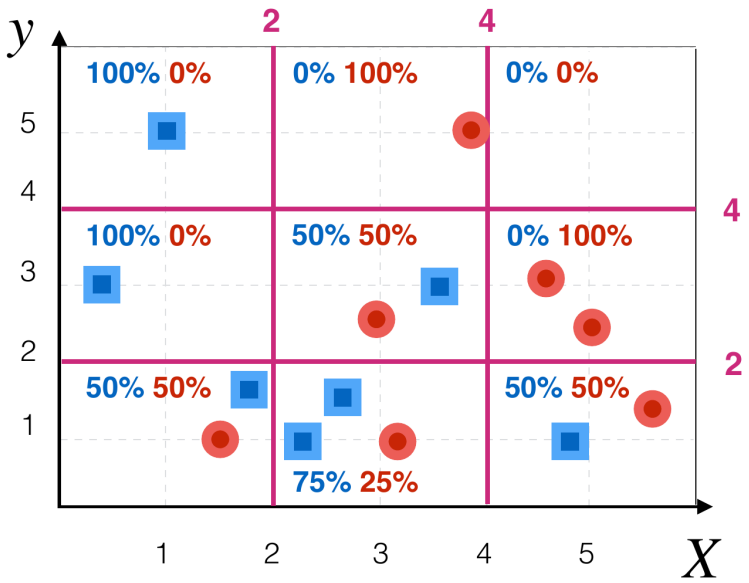

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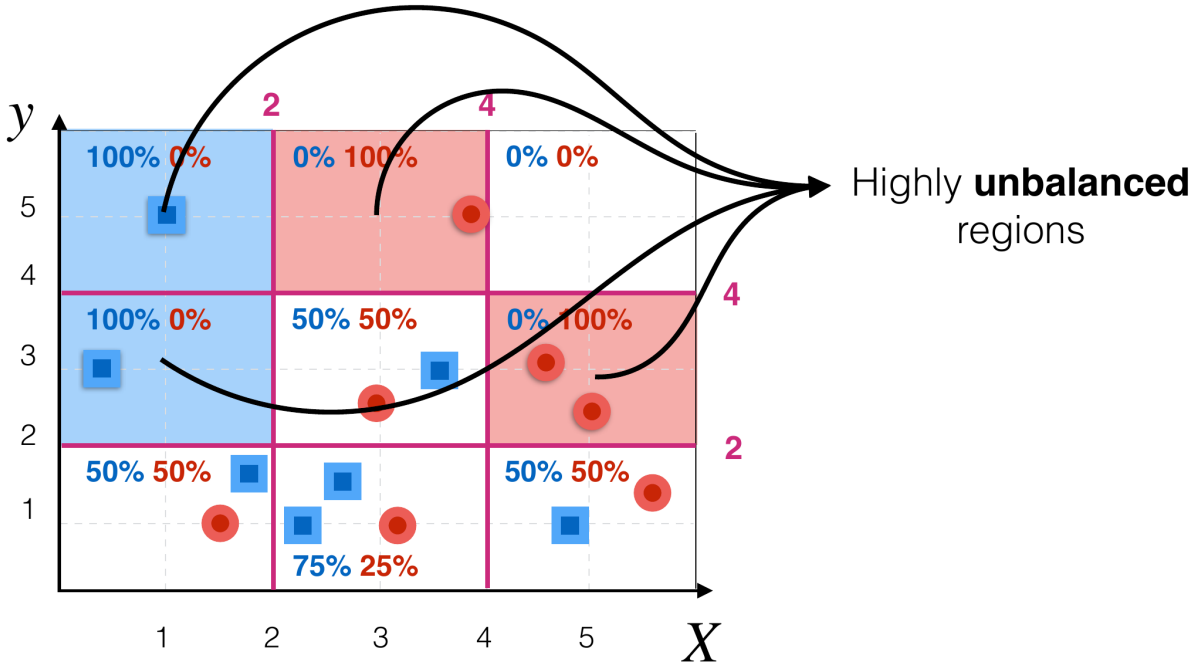

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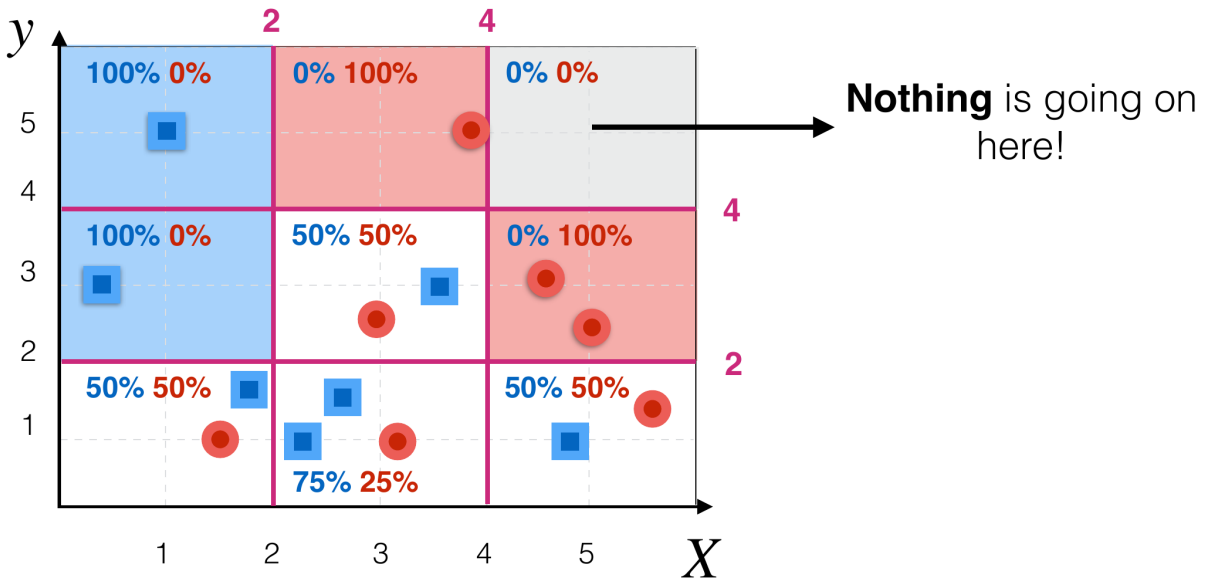

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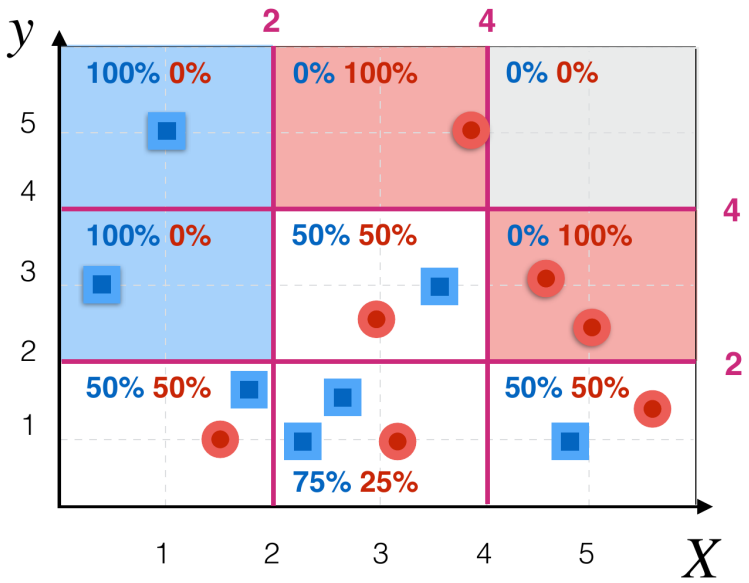

On average **55.5%** of cells will be either **empty** or **singletons**

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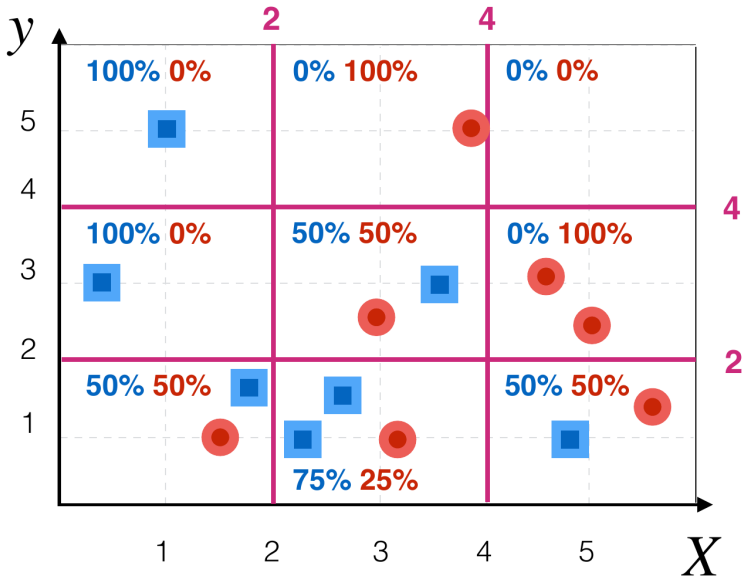

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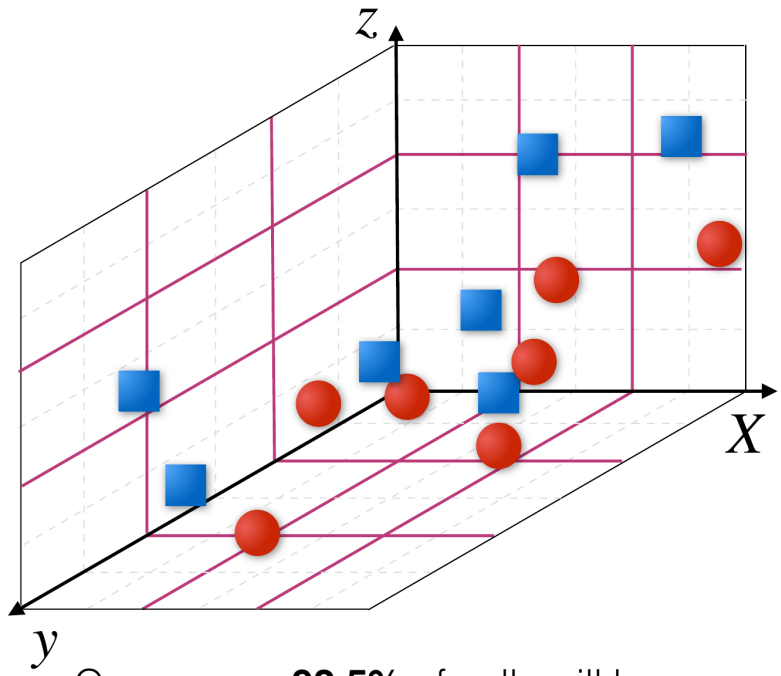
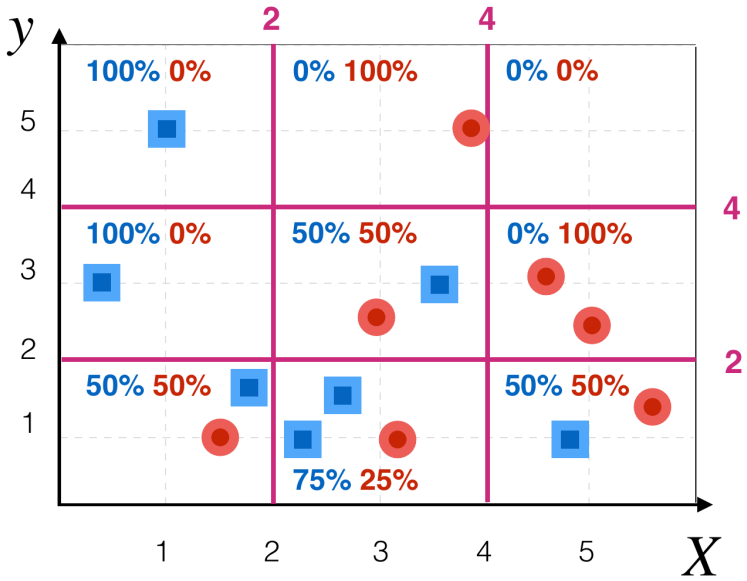


On average **92.5%** of cells will be either **empty** or **singletons**

What is the **curse** of **dimensionality**?

In order to keep **high-dimensional** space reasonably covered you need **a lot more data**



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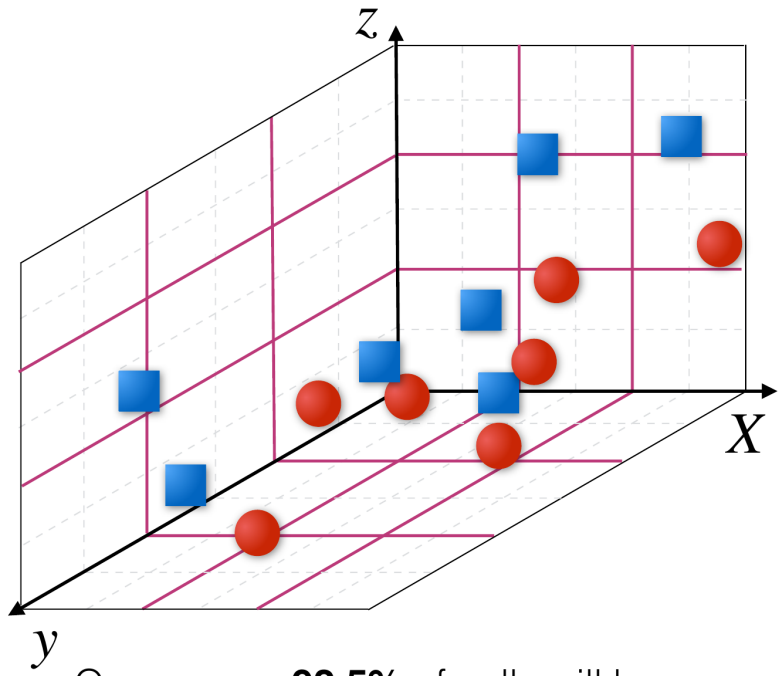

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Principal Component Analysis

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(part **II**)

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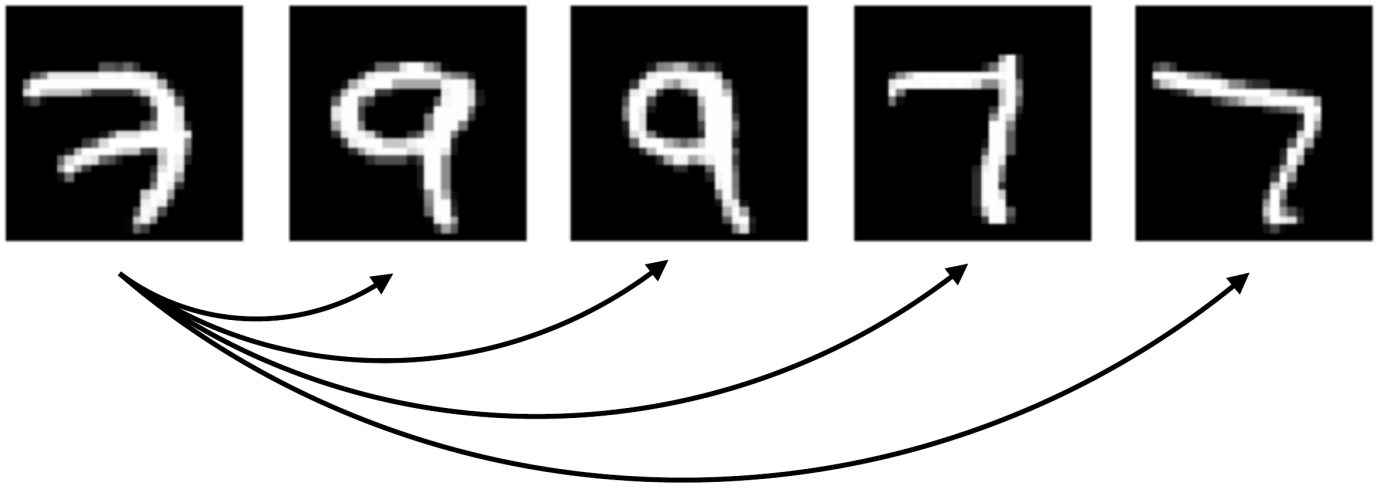
Distances become **similar** in high-dimensional space



Principal Component Analysis

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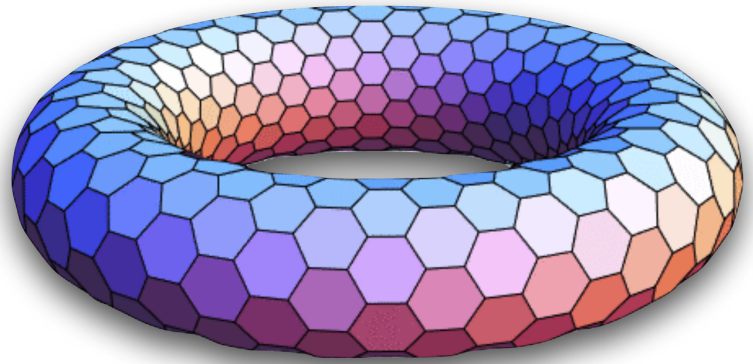

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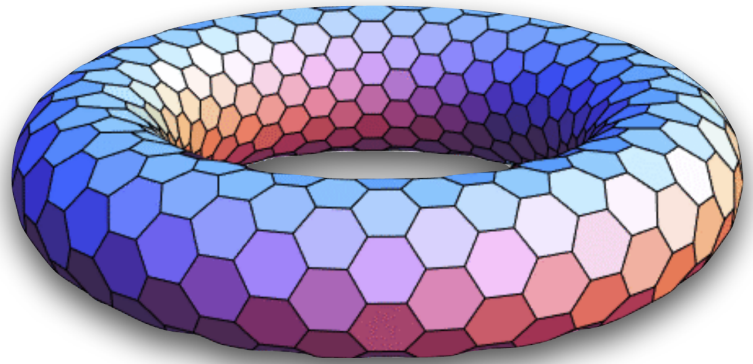
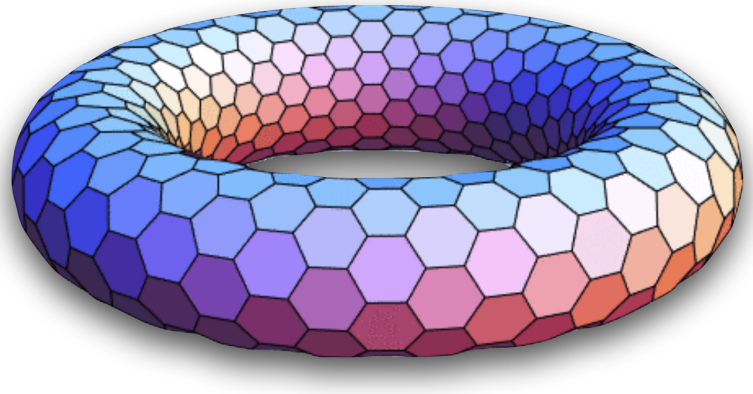


You need **more data** and **objects become closer** in high-dimensional space

Principal Component Analysis

Feature **extraction** vs feature **elimination**



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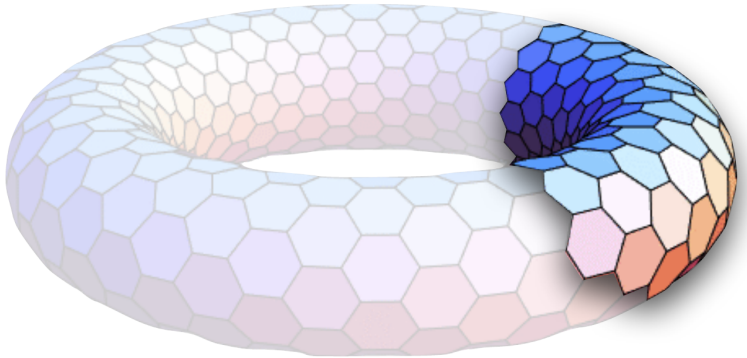

Keeping only **few** original **features**

Principal Component Analysis

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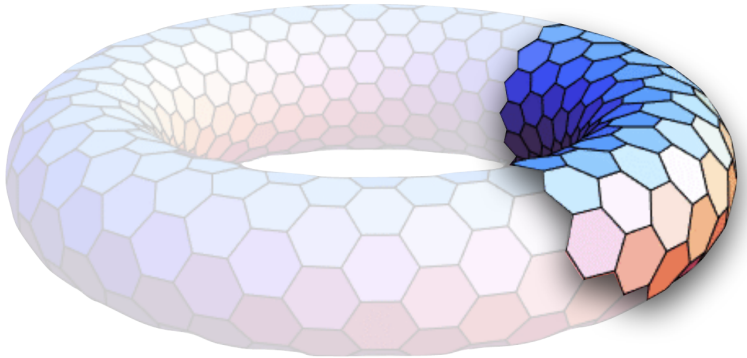

Remove
all **the rest**

Keeping only **few**
original **features**

Principal Component Analysis

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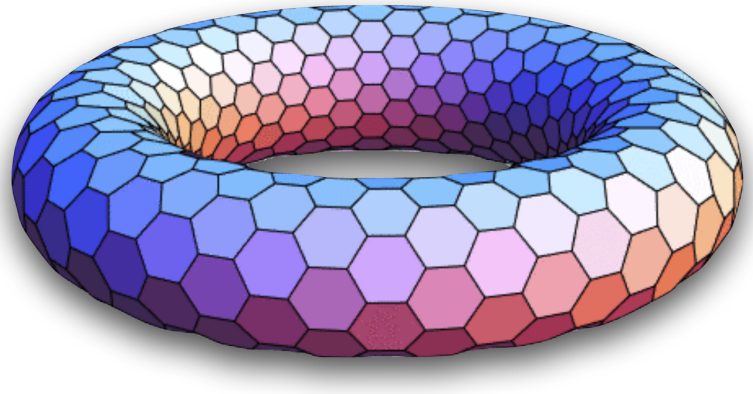

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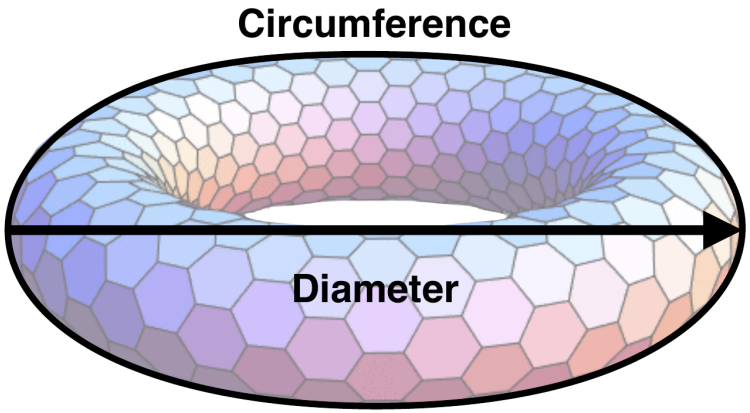

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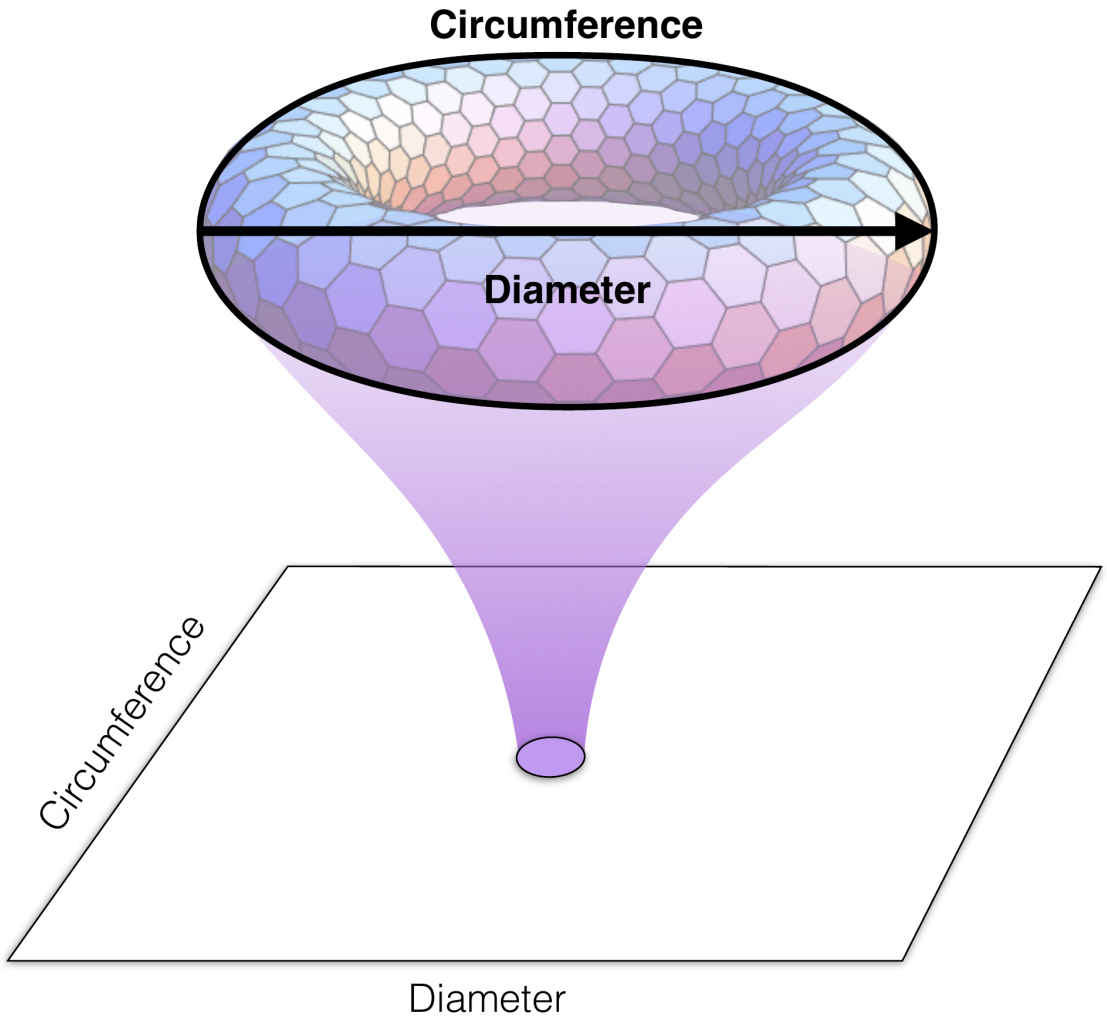

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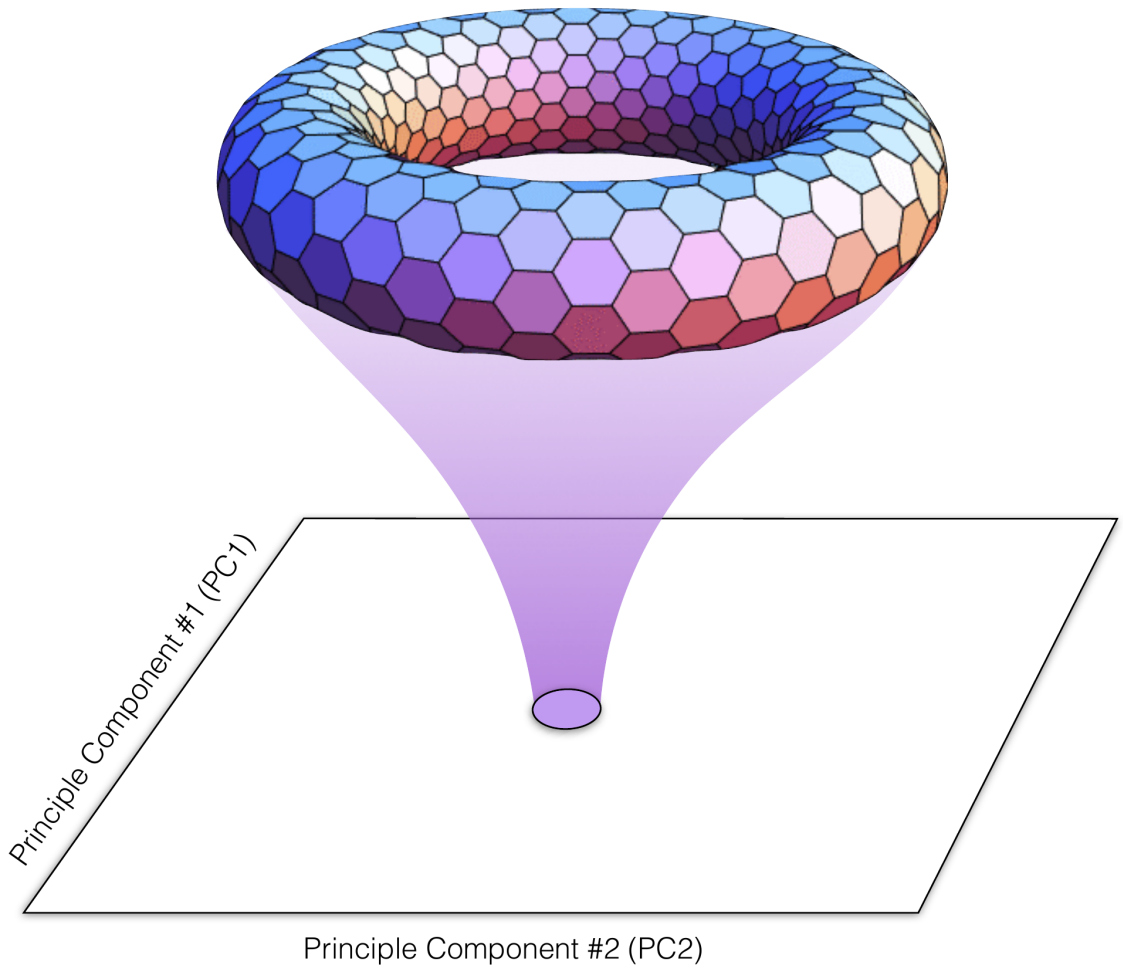
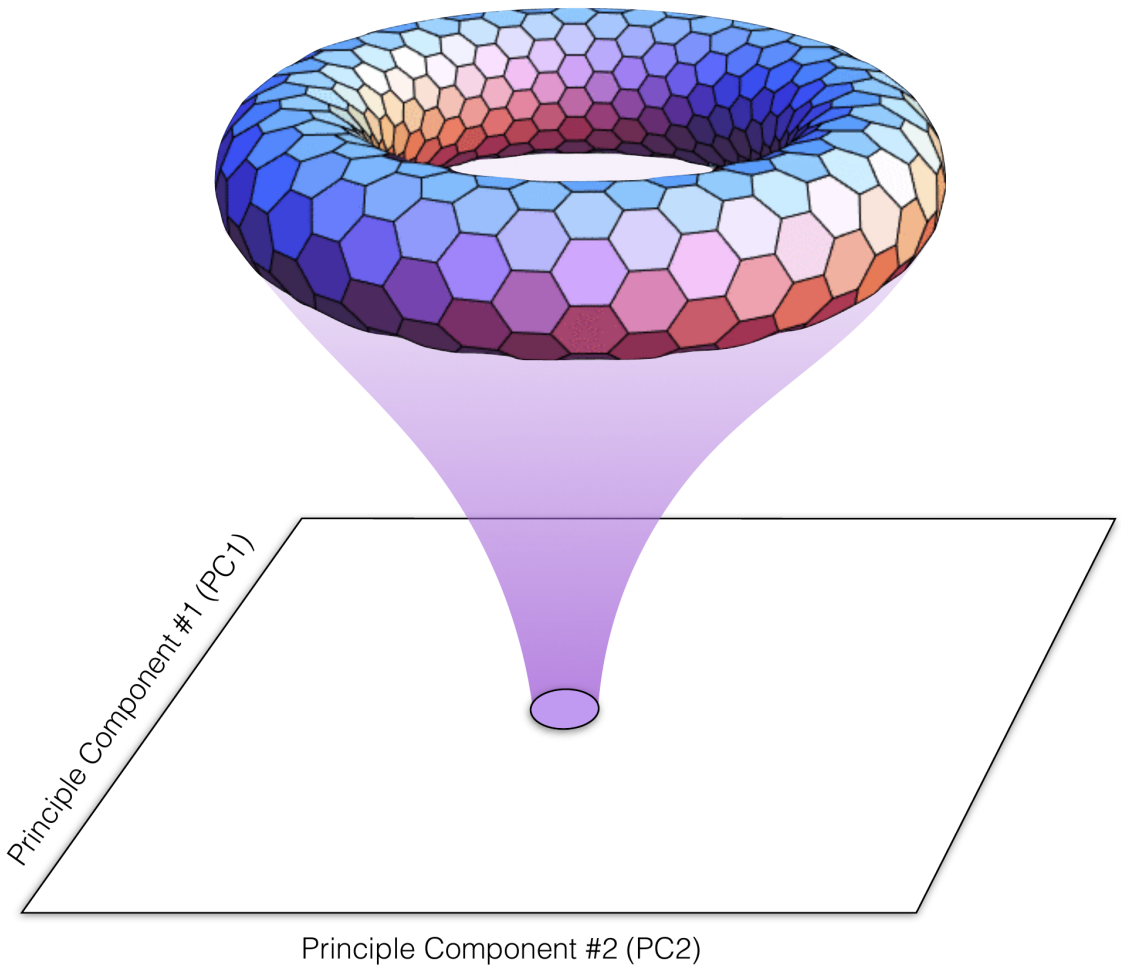
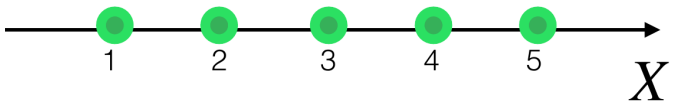


Principle **C**omponent **A**nalysis



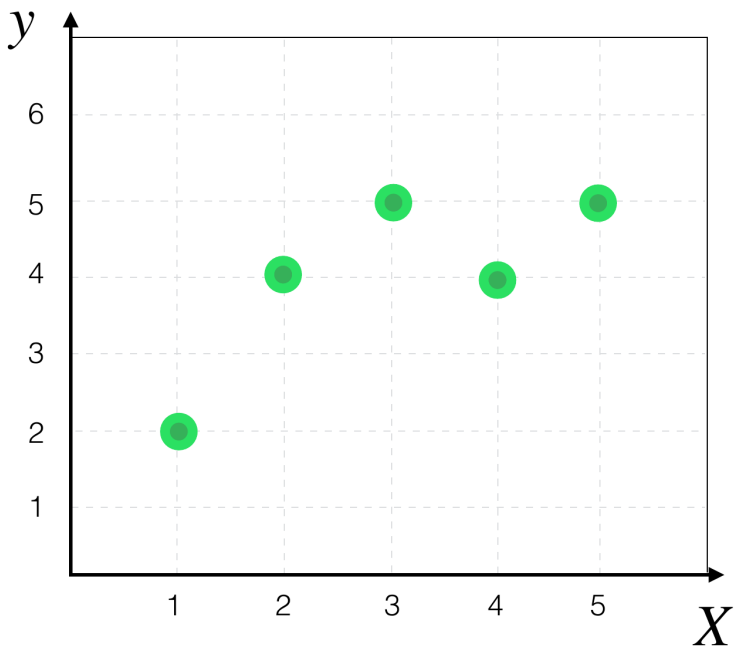
1-Dimensional data

x
1
2
3
4
5



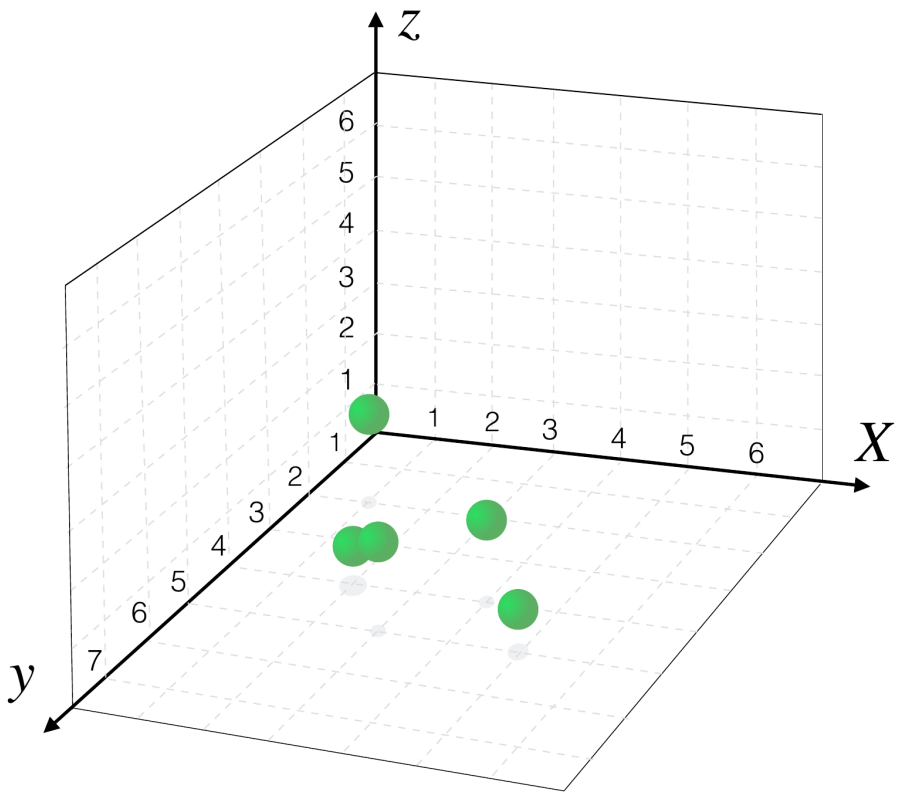
2-Dimensional data

x	y
1	2
2	4
3	5
4	4
5	5



3-Dimensional data

x	y	z
1	2	2
2	4	0.5
3	5	1
4	4	1
5	5	0.5



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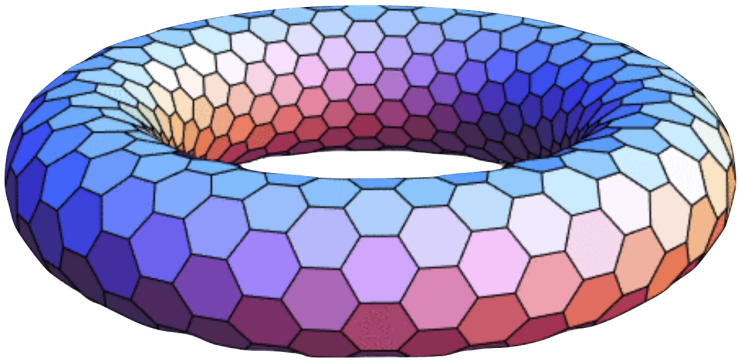
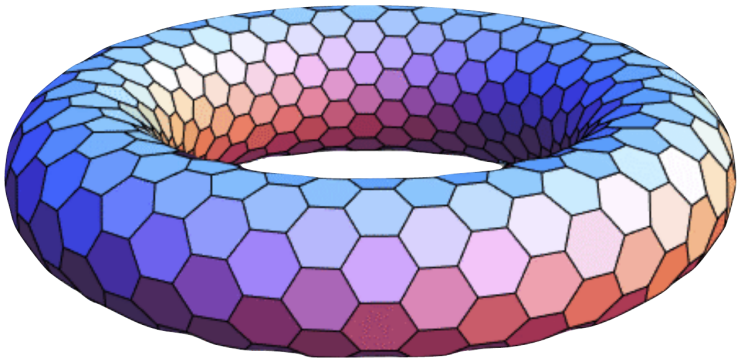


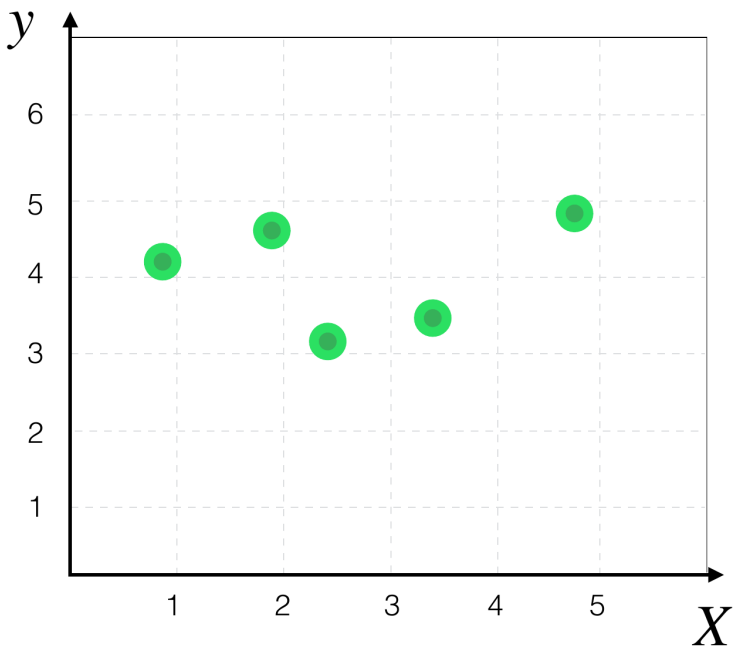
200-Dimensional data?



200-Dimensional data?

Are all of these dimensions **equally useful**?

2-D example revisited



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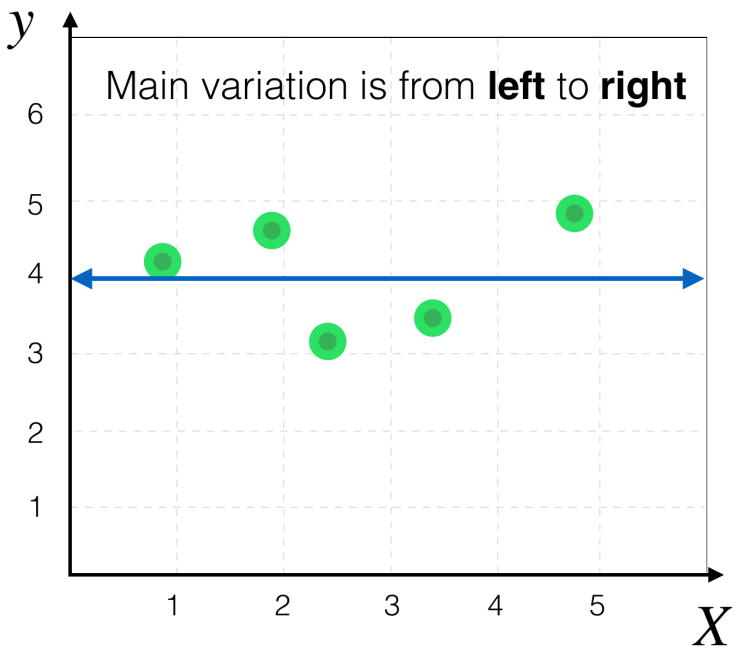

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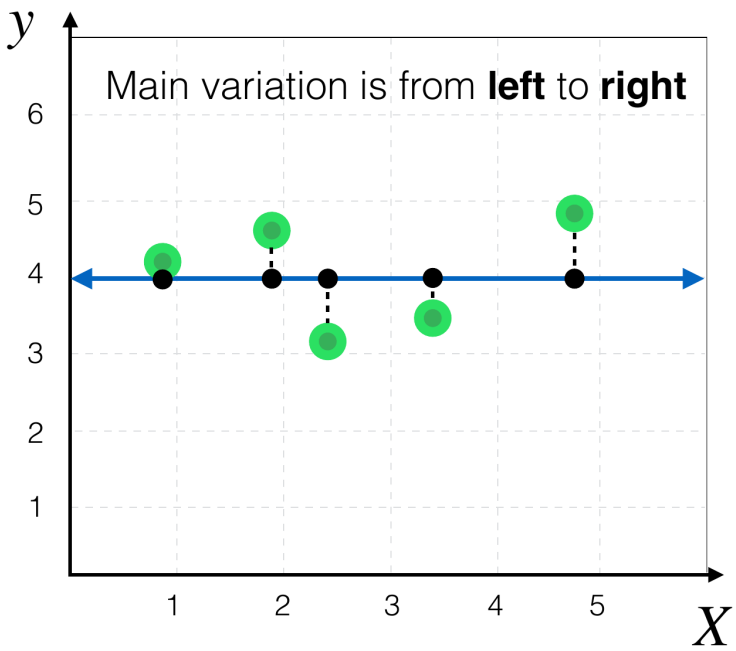

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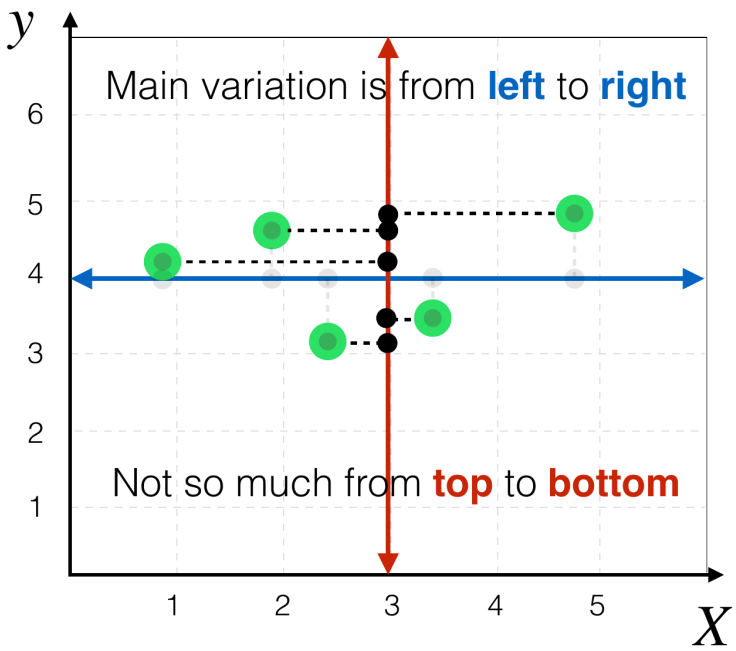

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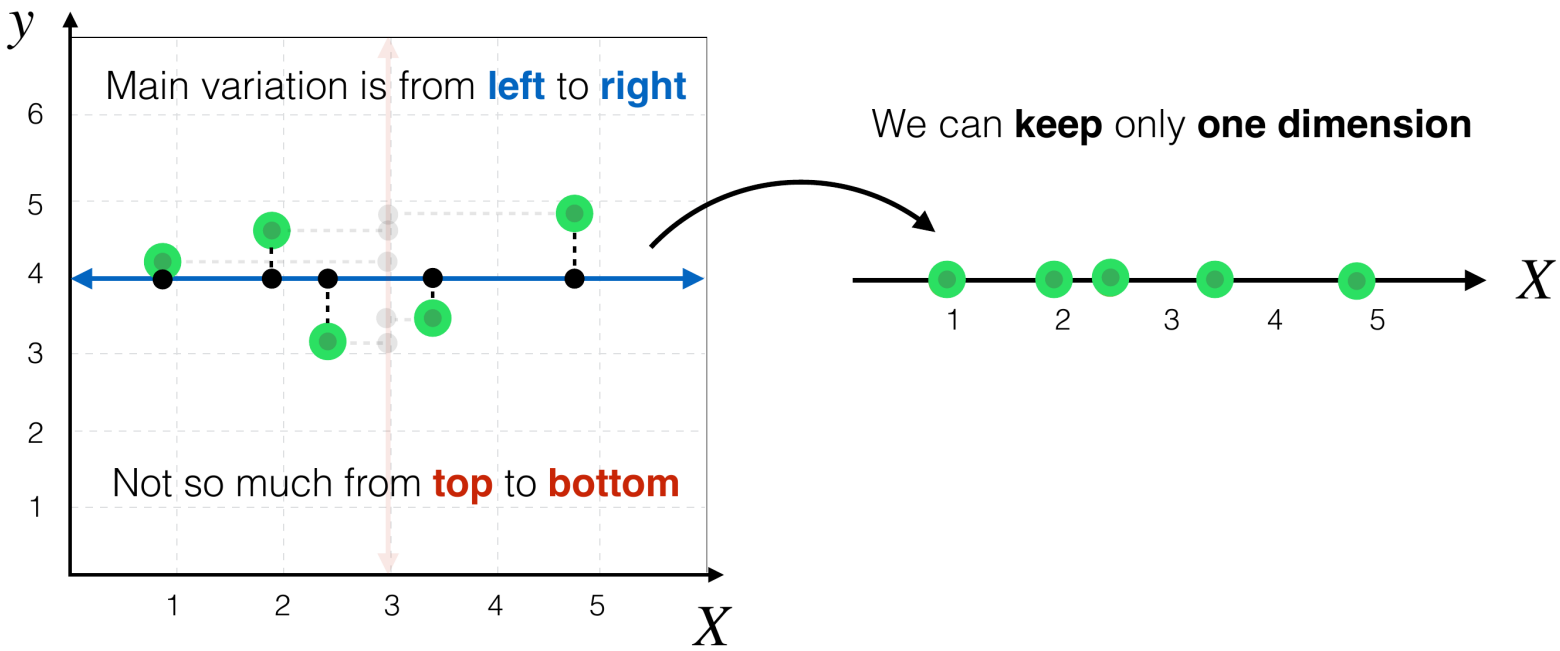

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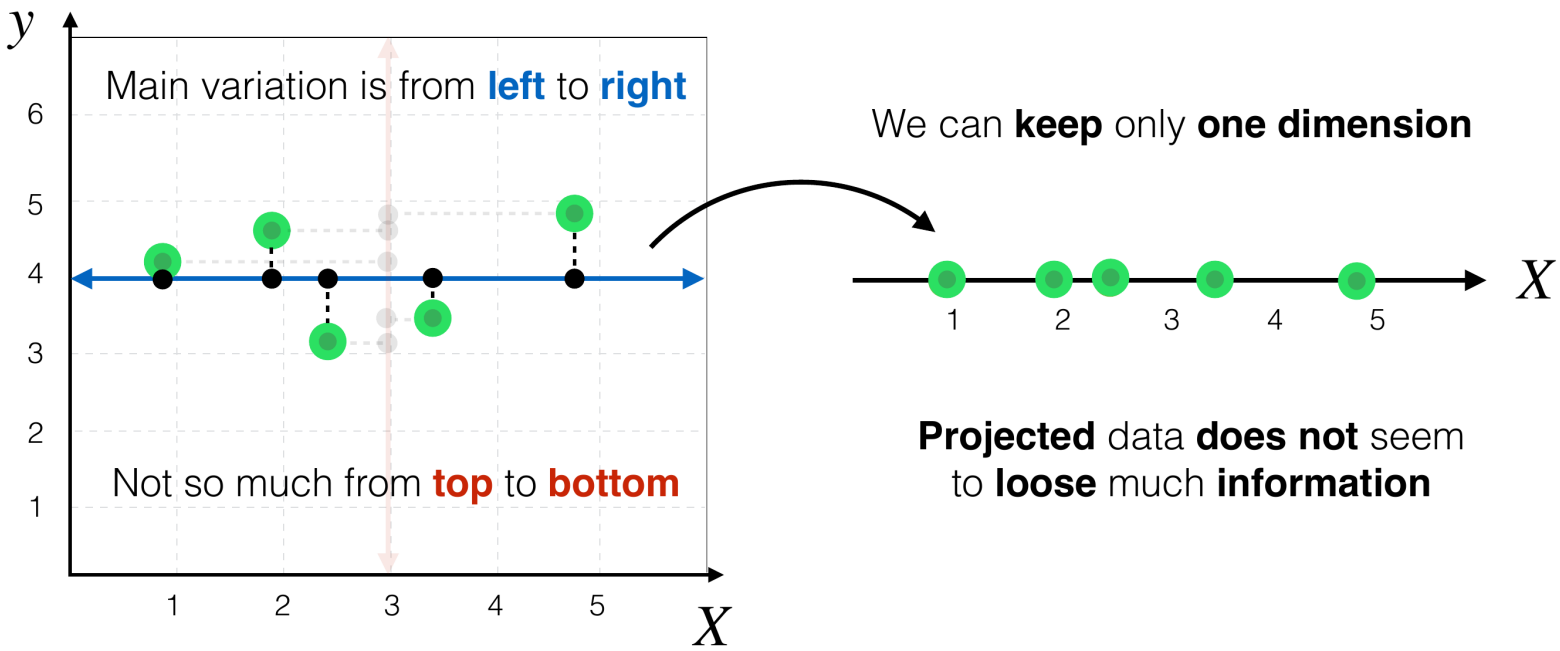

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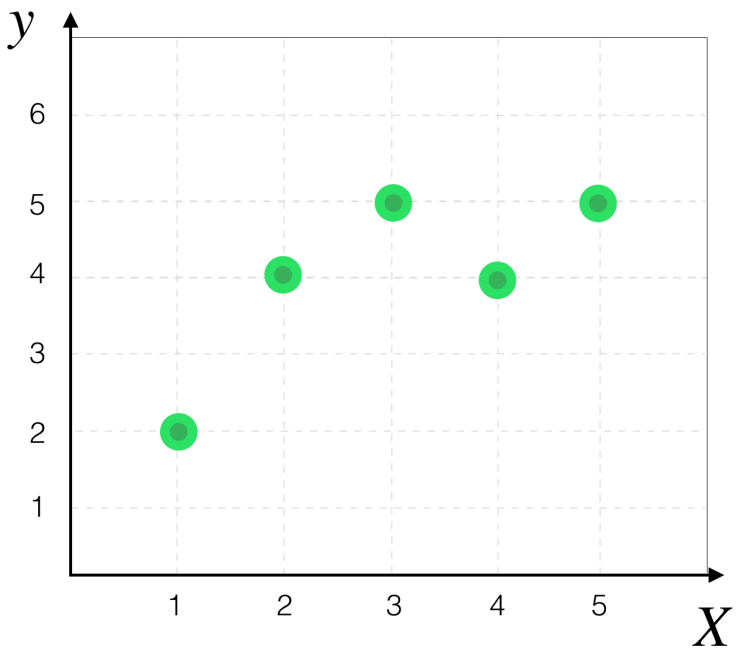

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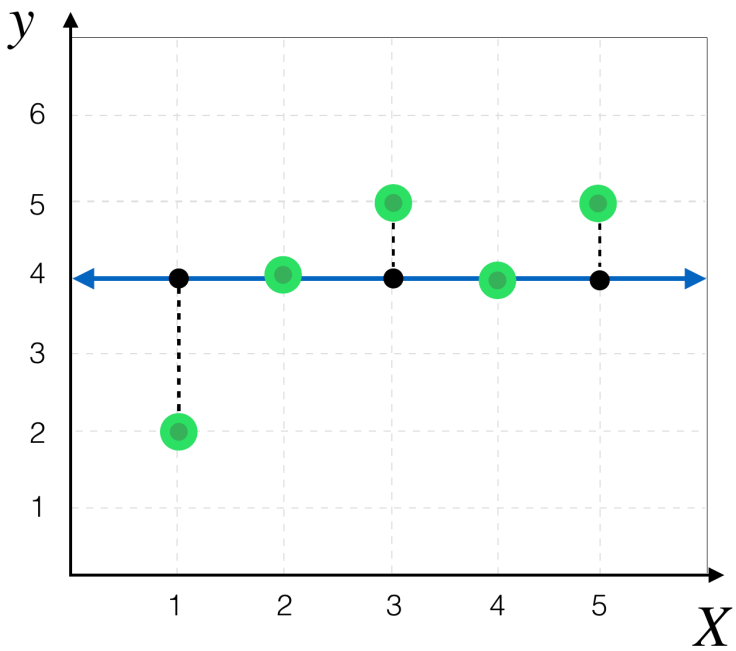
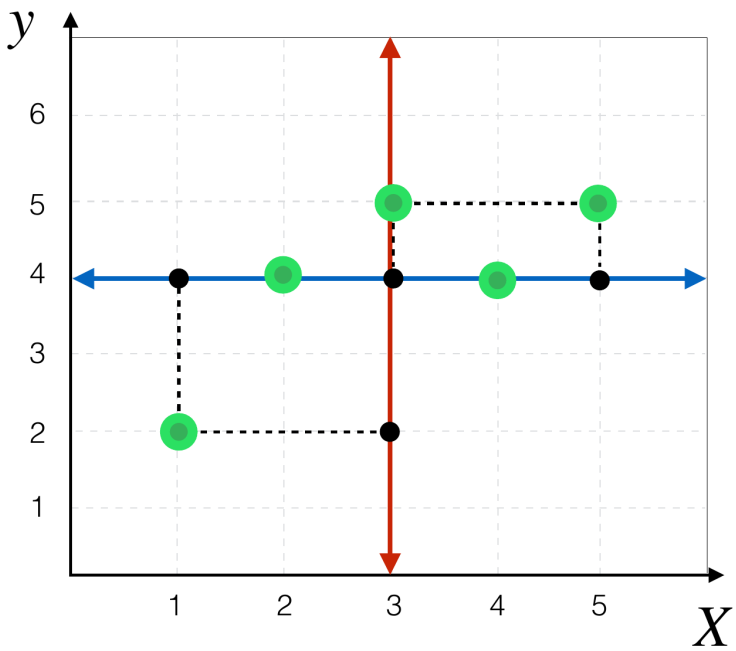
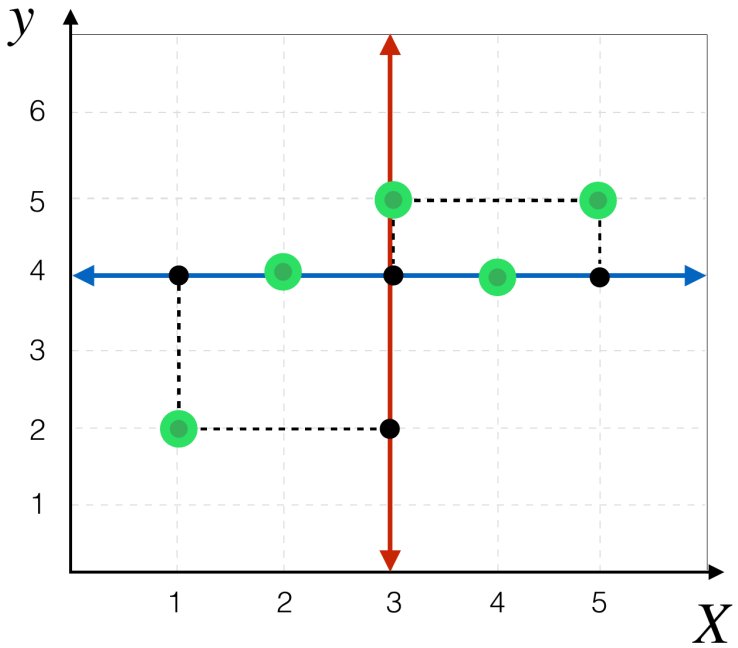


2-D example revisited

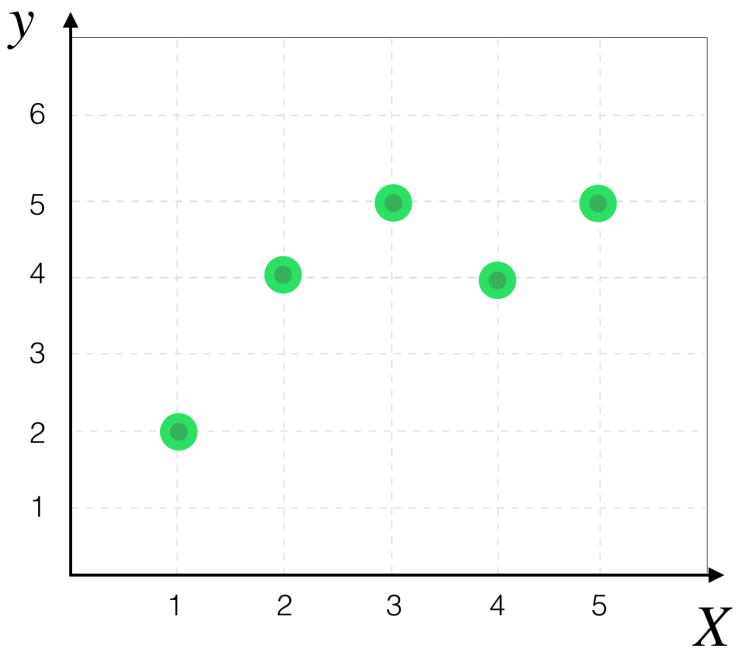


2-D example revisited

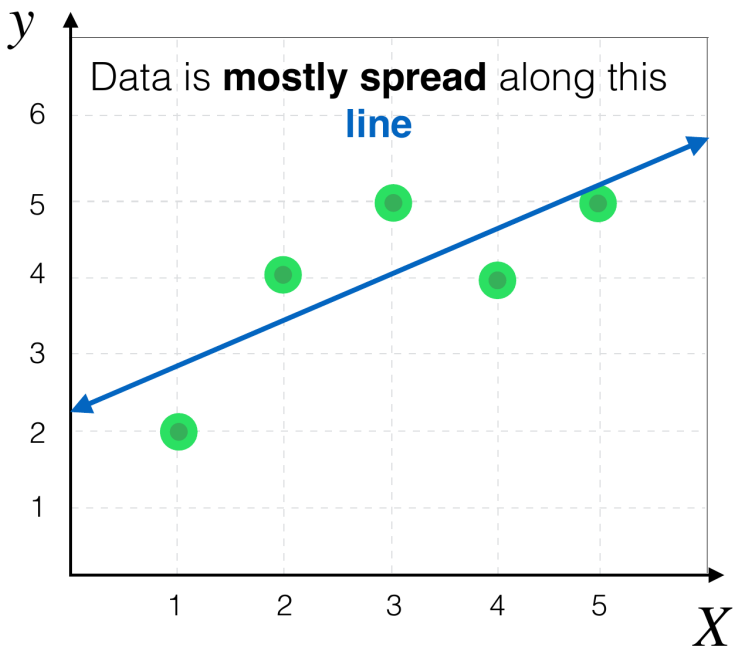
Data seem to be **spread more equally** along **X** and **y** axes



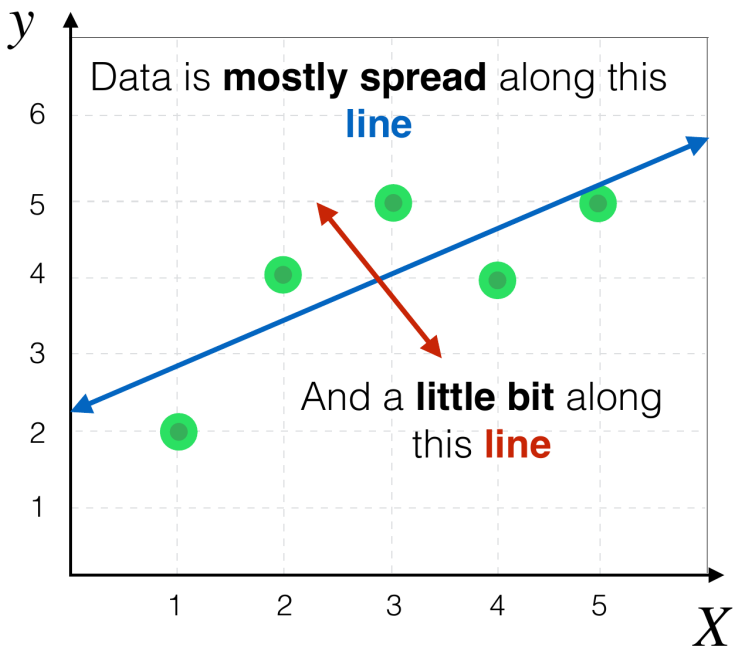
2-D example revisited



2-D example revisited

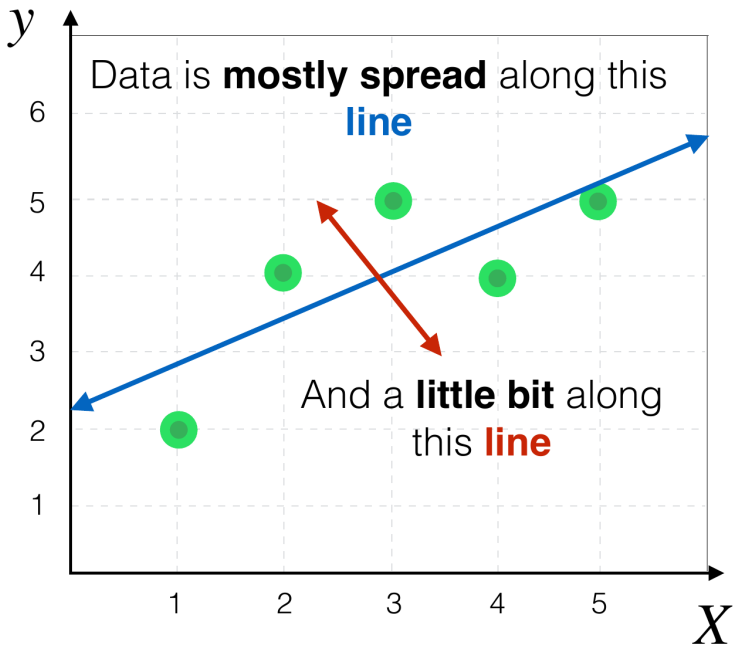


2-D example revisited



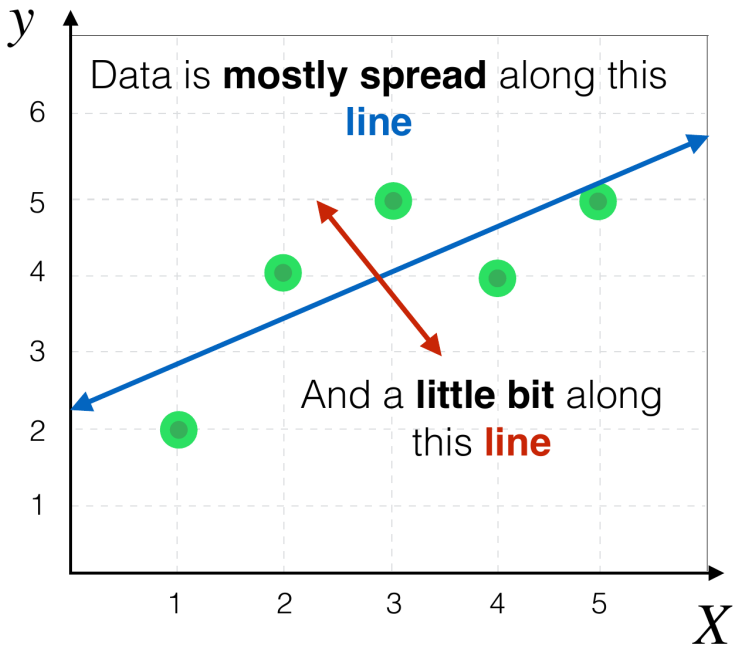
2-D example revisited

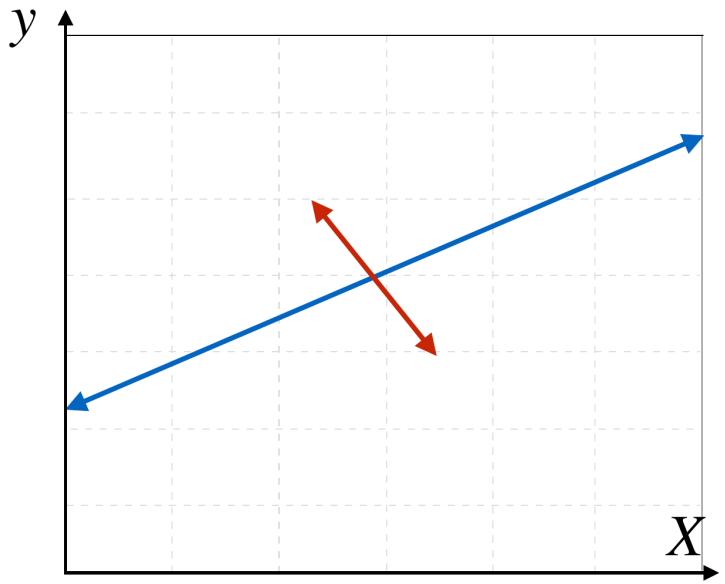
How about we make **new axes** from **these lines**?



2-D example revisited

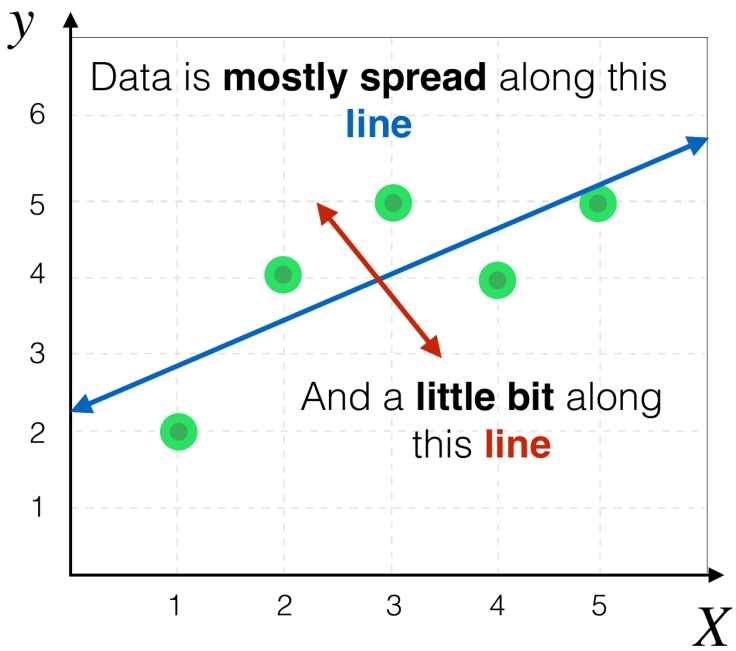
How about we make **new axes** from **these lines**?

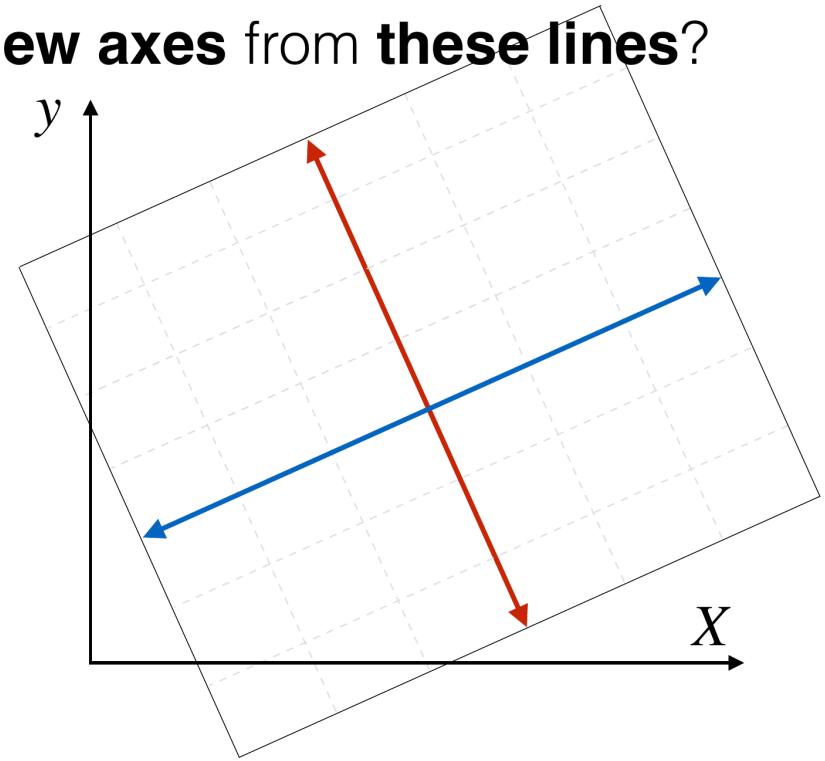




2-D example revisited

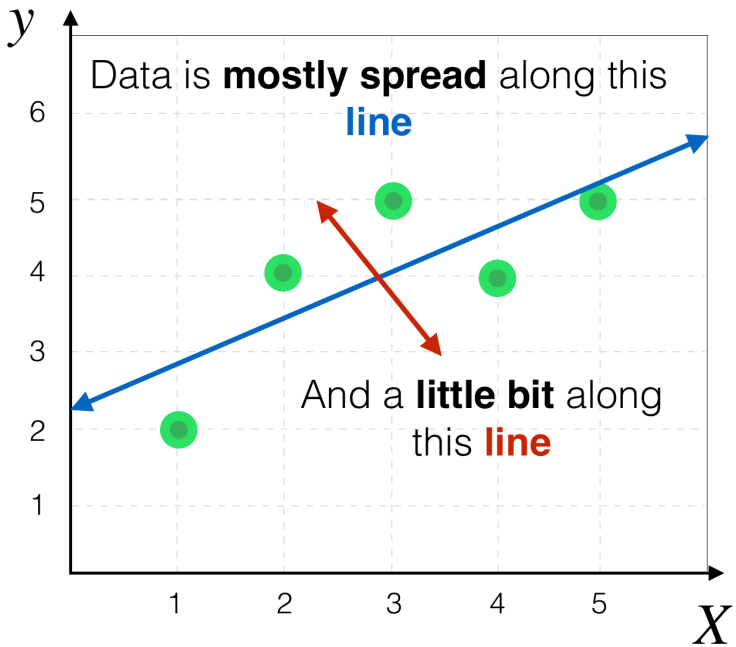
How about we make **new axes** from **these lines**?

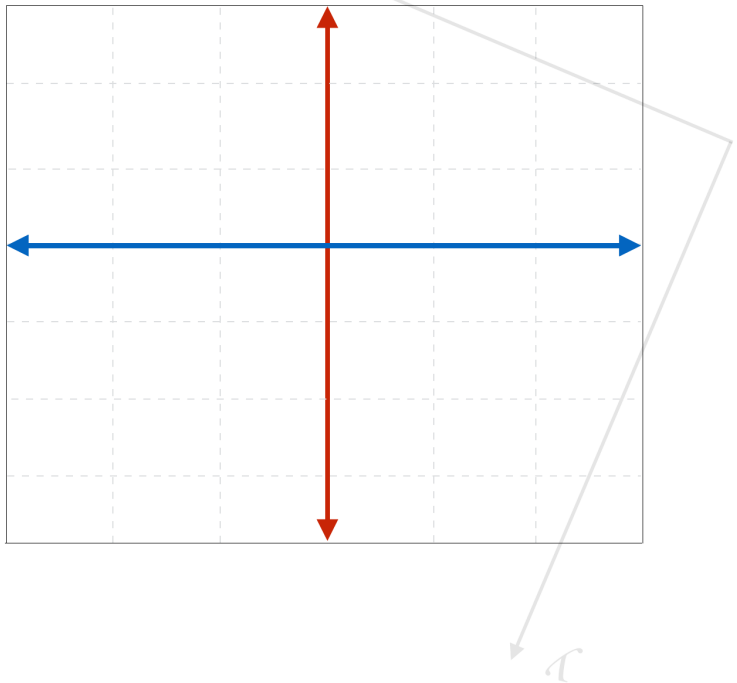




2-D example revisited

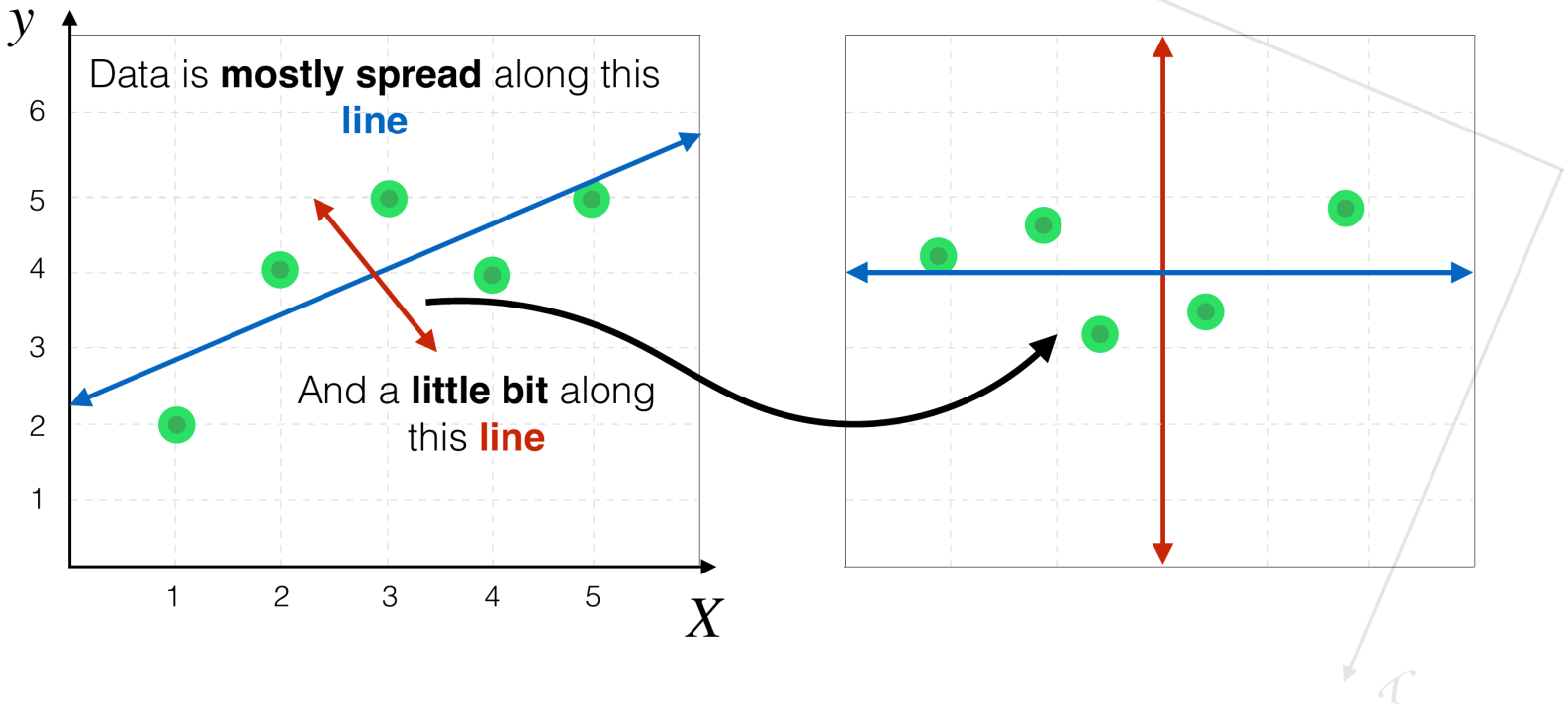
How about we make **new axes** from **these lines**?





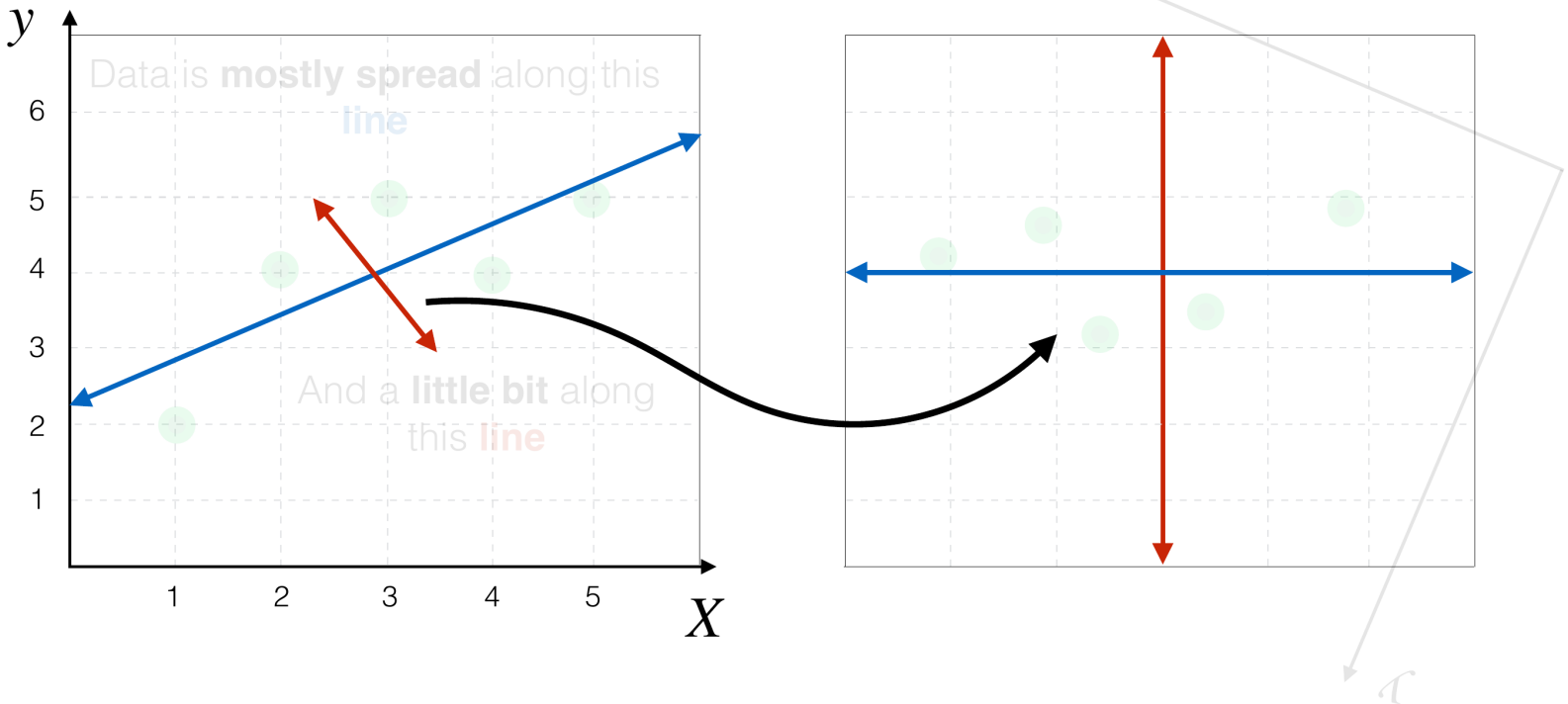
2-D example revisited

How about we make **new axes** from **these lines**?



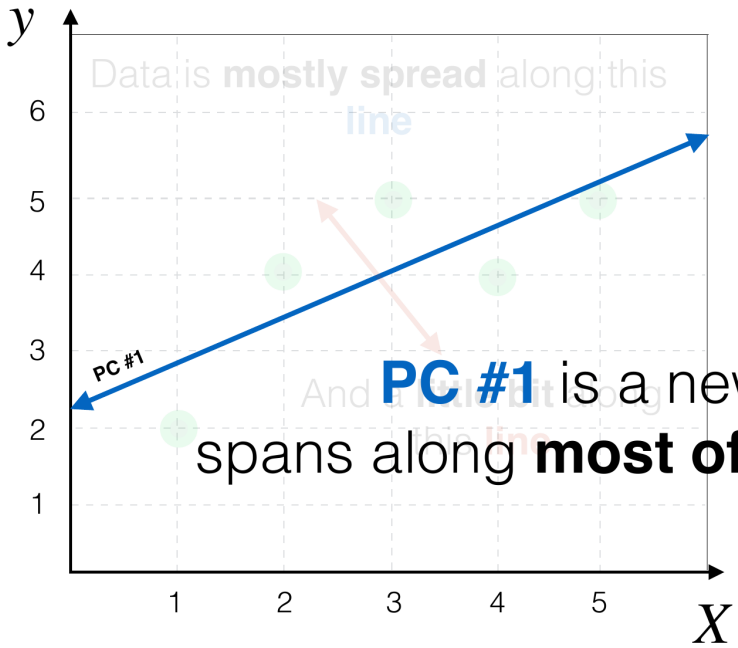
2-D example revisited

These **new axes** are called principle components



2-D example revisited

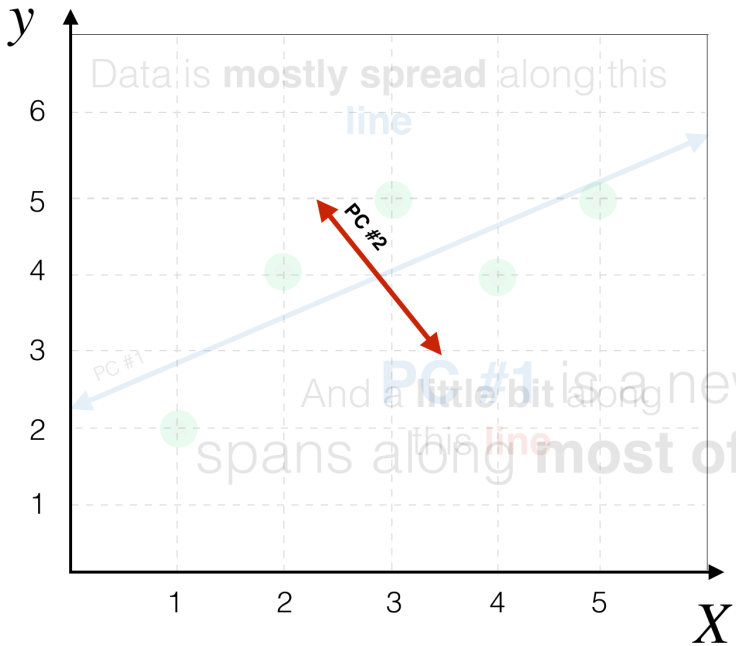
These **new axes** are called principle components

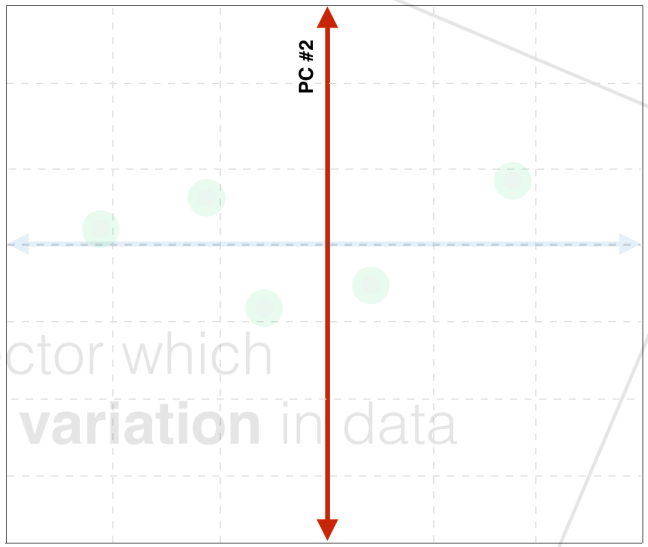


PC #1 is a new vector which spans along **most of the variation** in data

2-D example revisited

These **new axes** are called principle components

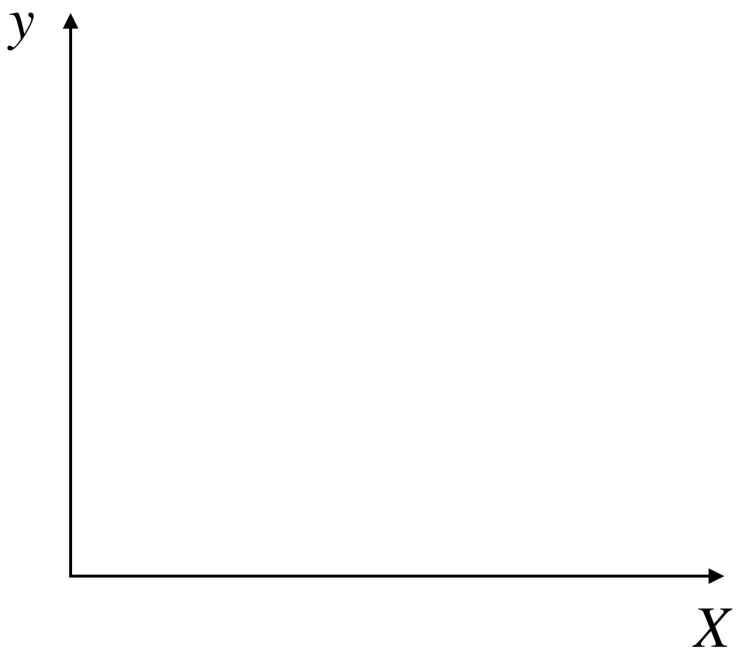


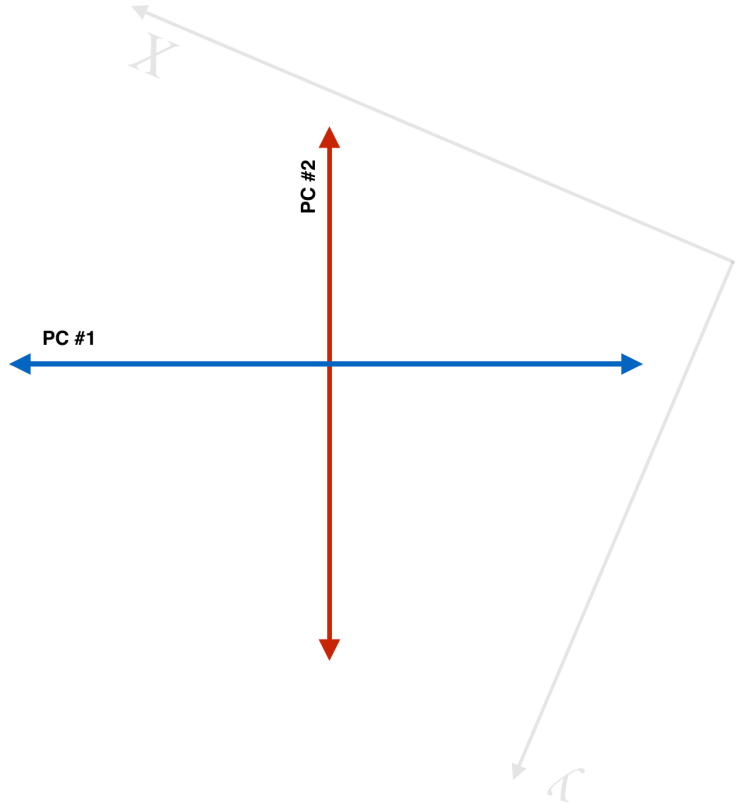


PC #2 is another new vector which spans along the direction of the second most variation

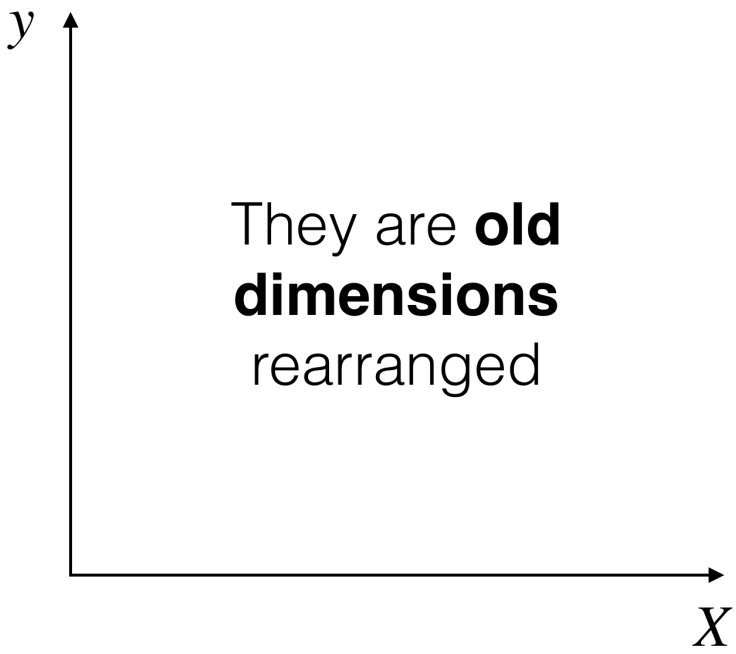
Principal Component Analysis

Principle components are **not additional axes/dimensions**

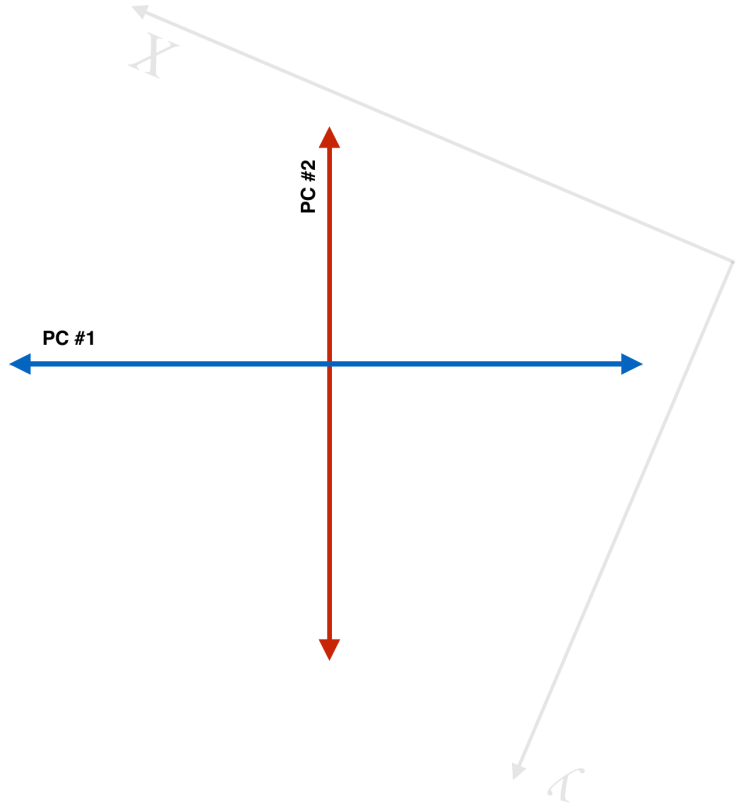




Principle components are **not additional axes/dimensions**

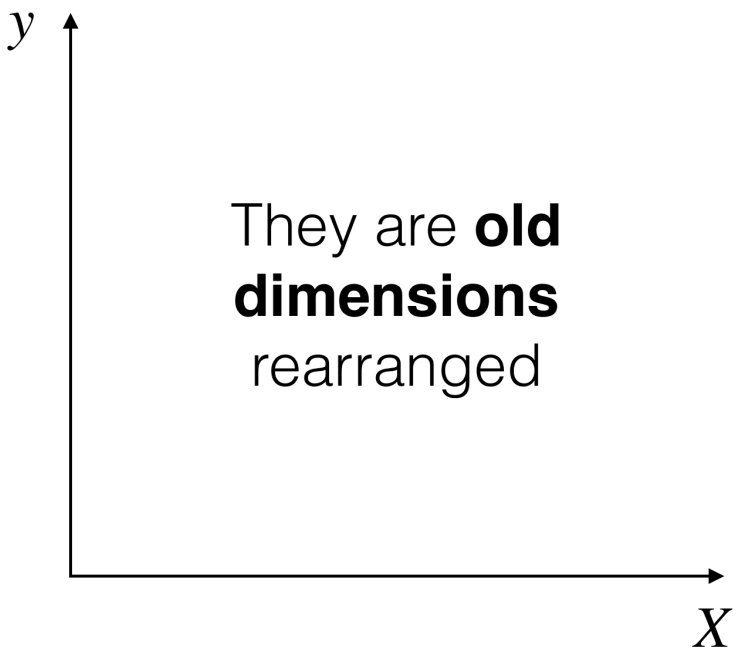


They are **old dimensions** rearranged

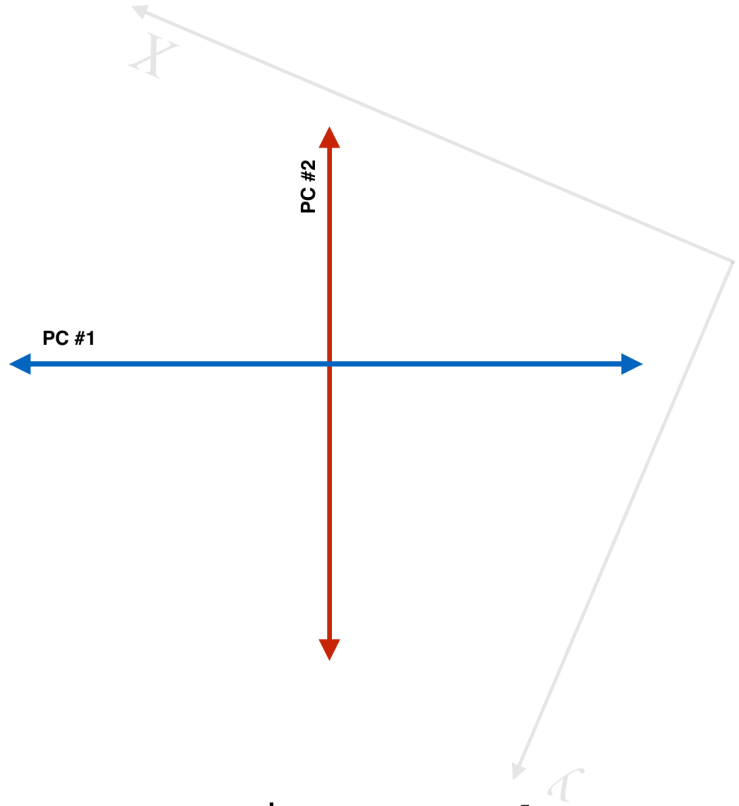


Principal Component Analysis

Principle components are **not additional axes/dimensions**

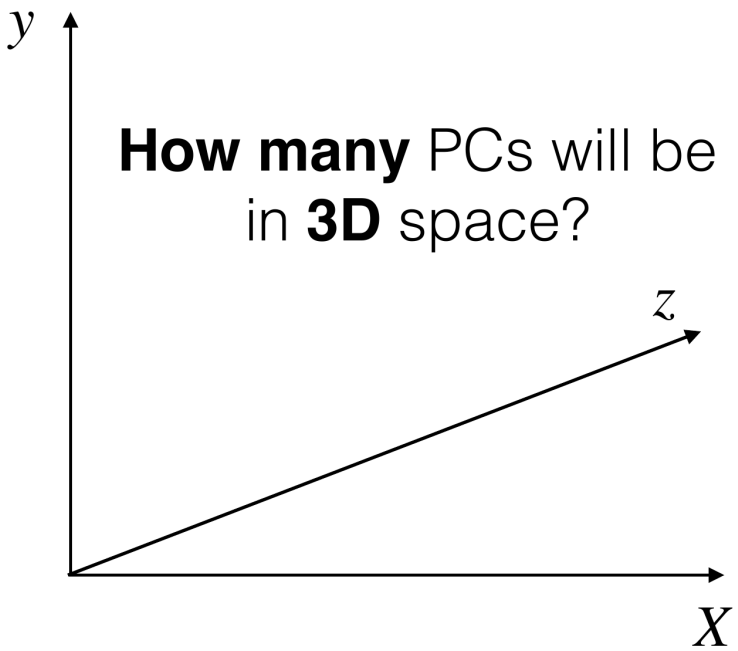


They are **old dimensions** rearranged



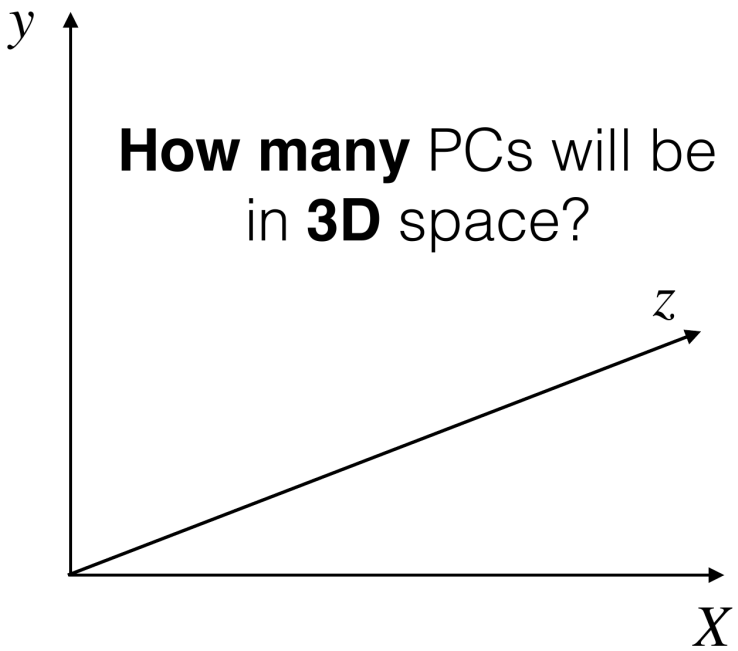
Such that the **first axis** now spans along **most variation**, the **second** the **second most variation** etc.

Principle components are **not additional axes/dimensions**

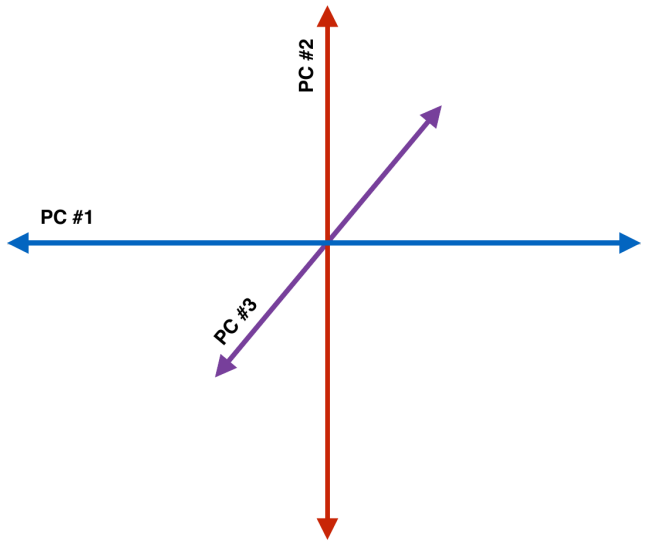


Principal Component Analysis

Principle components are **not additional axes/dimensions**



How many PCs will be in **3D** space?

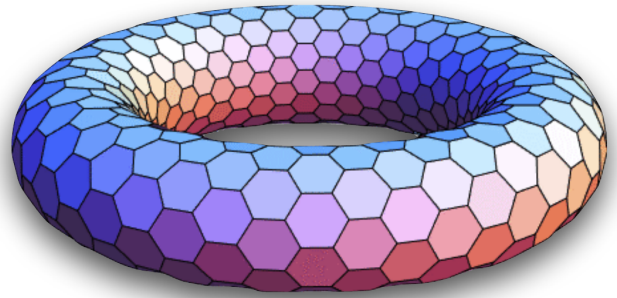


As many as there were **original dimensions**, hence **3** PCs

Principal Component Analysis

Principle components are **not additional axes/dimensions**

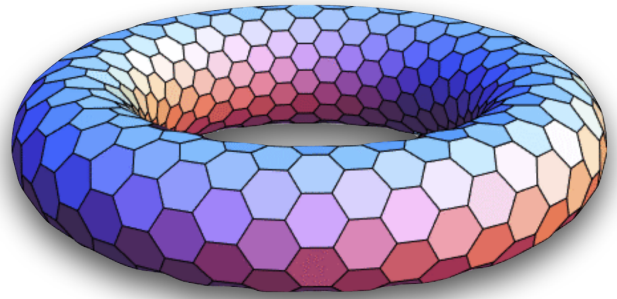
How many PCs will be formed in **200D** space?

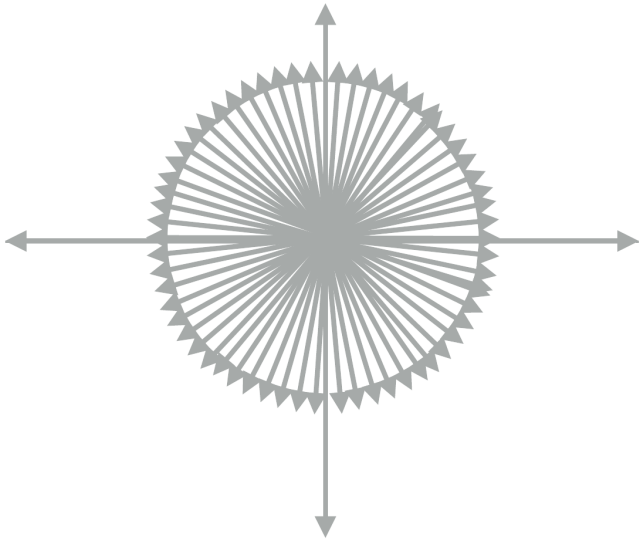


Principal Component Analysis

Principle components are **not additional axes/dimensions**

How many PCs will be formed in **200D** space?



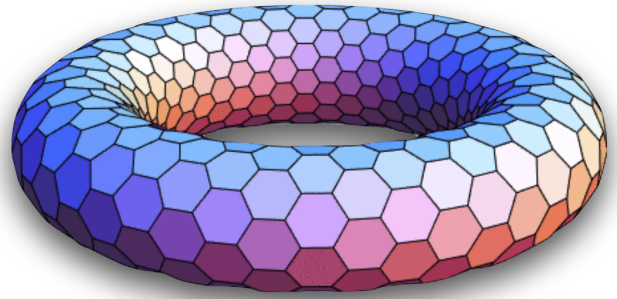


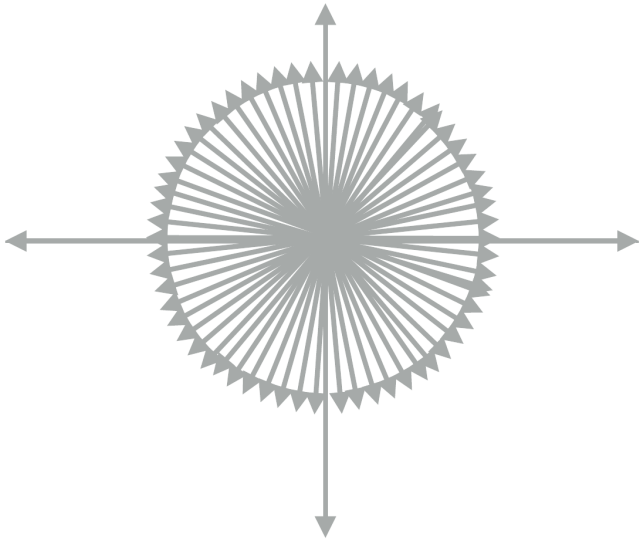
No exceptions, **200 PCs**

Principal Component Analysis

Principle components are **not additional axes/dimensions**

How many PCs will be formed in **200D** space?

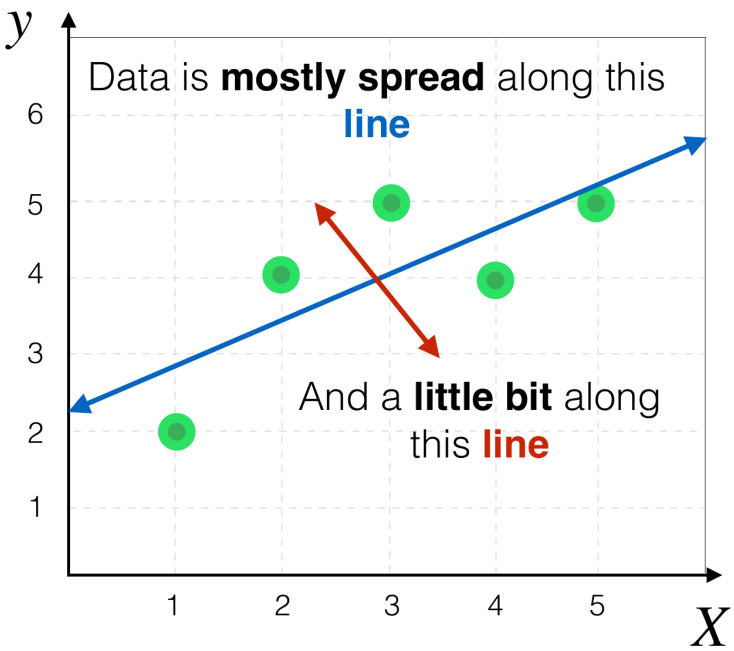


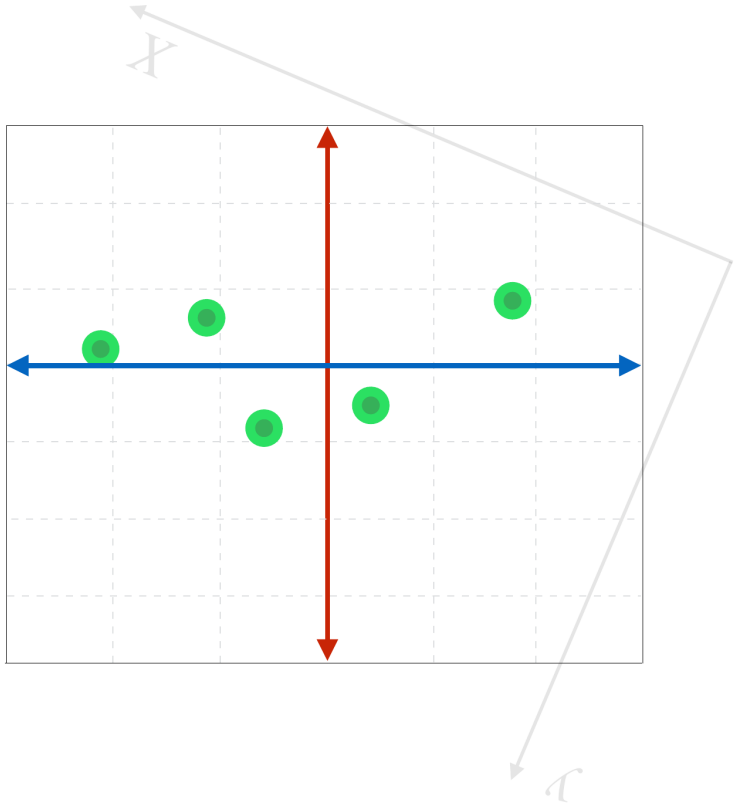


No exceptions, **200 PCs**

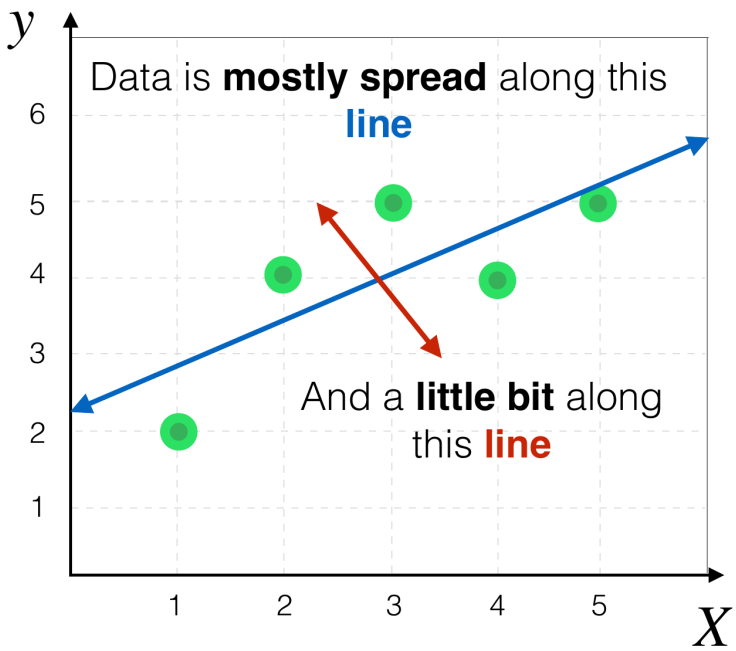
But what is **the benefit** of having PCs?

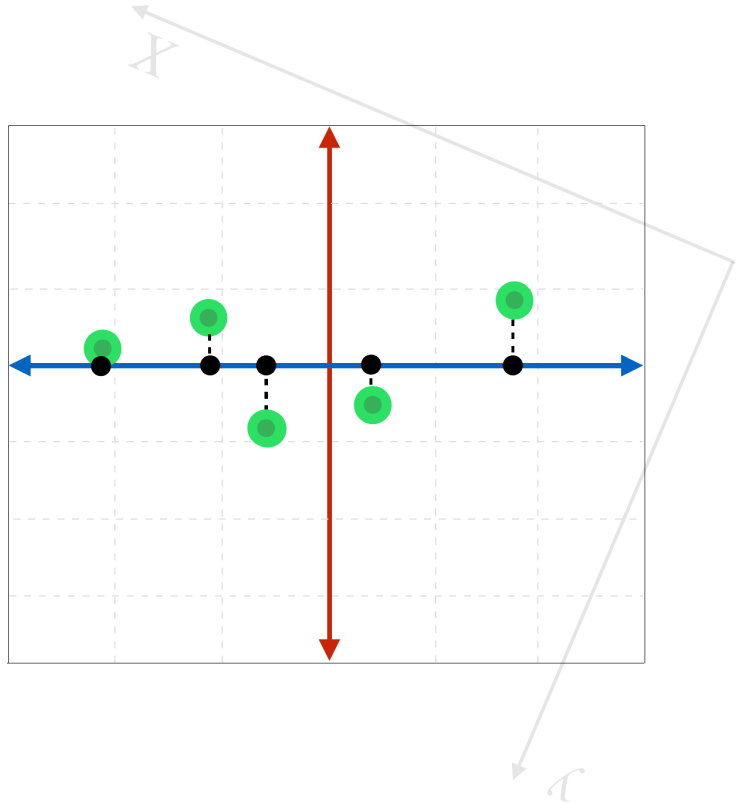
Principal Component Analysis



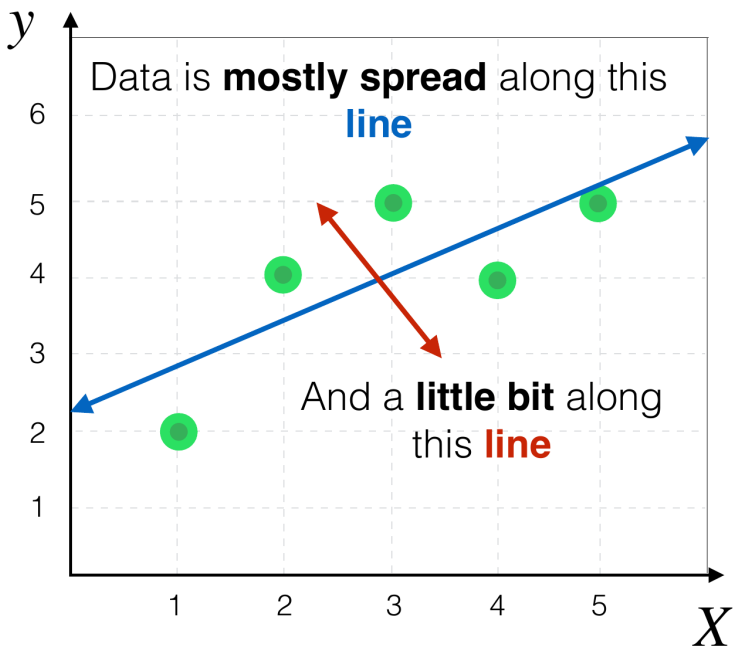


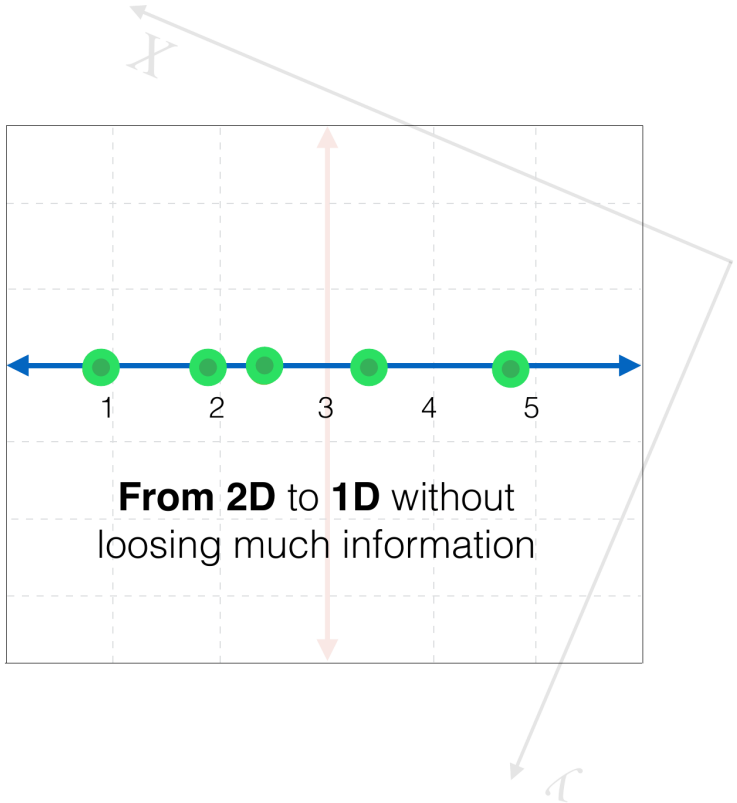
Principal Component Analysis





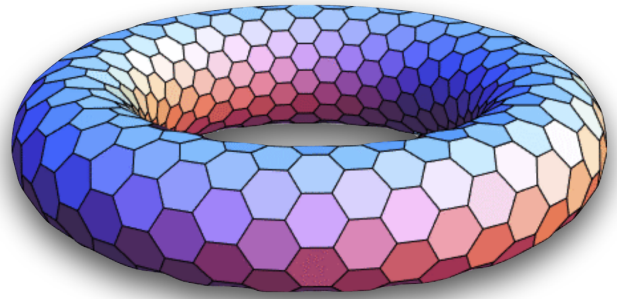
Principal Component Analysis

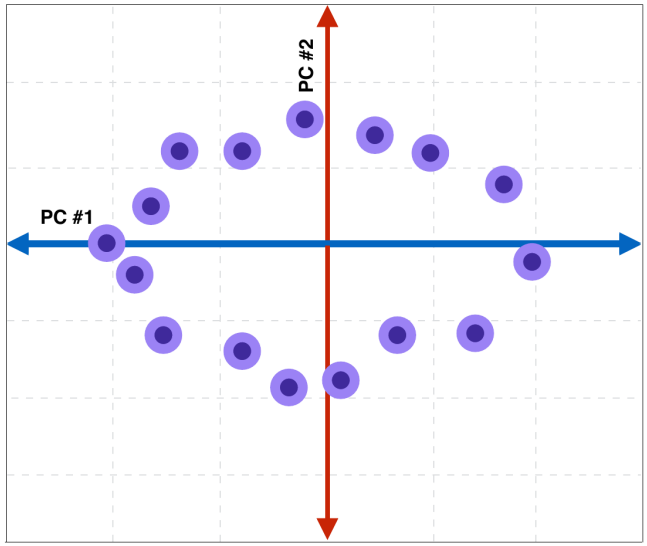




Principle components are **not additional axes/dimensions**

How many PCs will be formed in **200D** space?





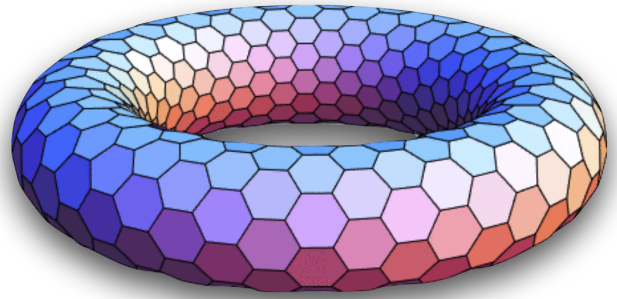
No exceptions, **200 PCs**

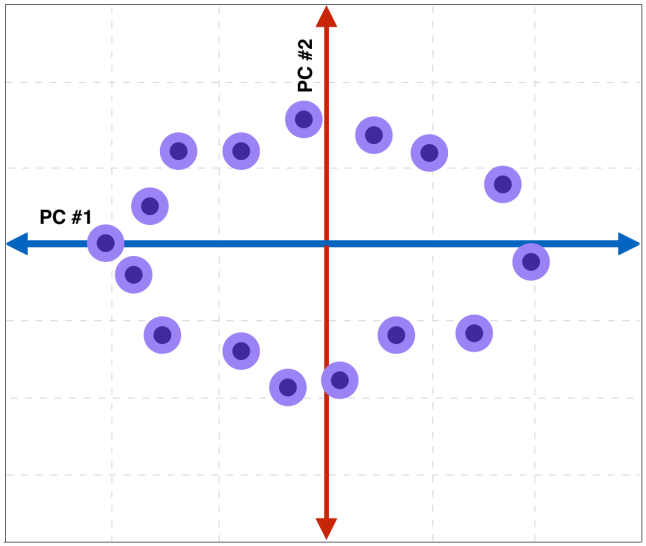
But what is **the benefit** of having PCs?

Principal Component Analysis

Principle components are **not additional axes/dimensions**

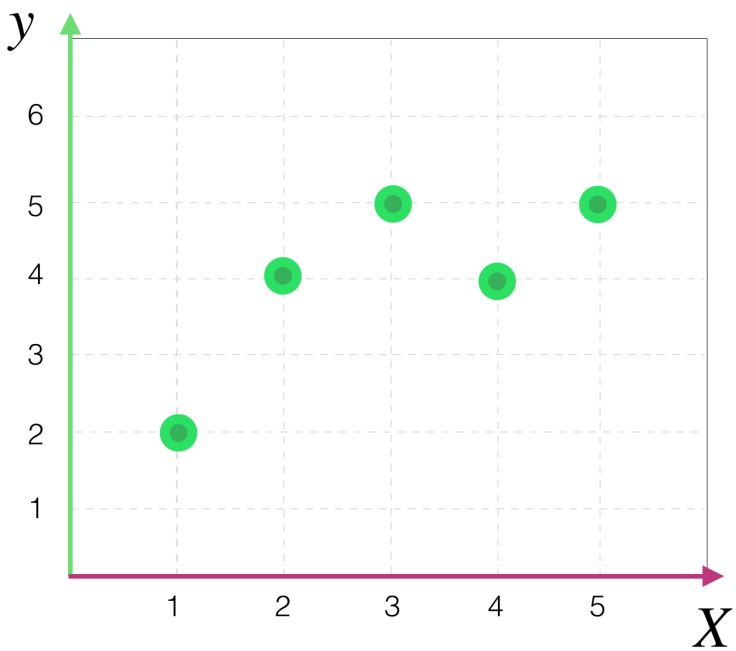
How many PCs will be formed in **200D** space?





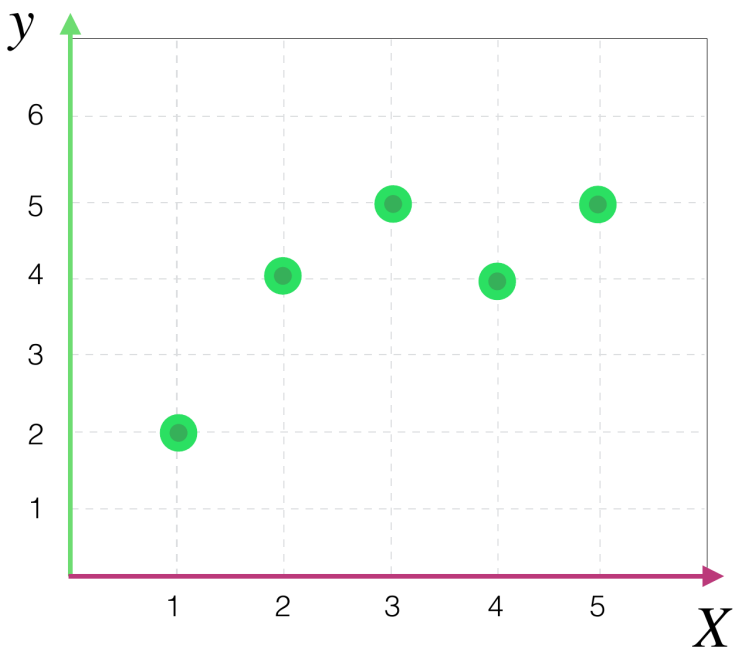
First few PCs would be **enough** to capture important information

Principal Component Analysis



x	y
1	2
2	4
3	5
4	4
5	5

Principal Component Analysis

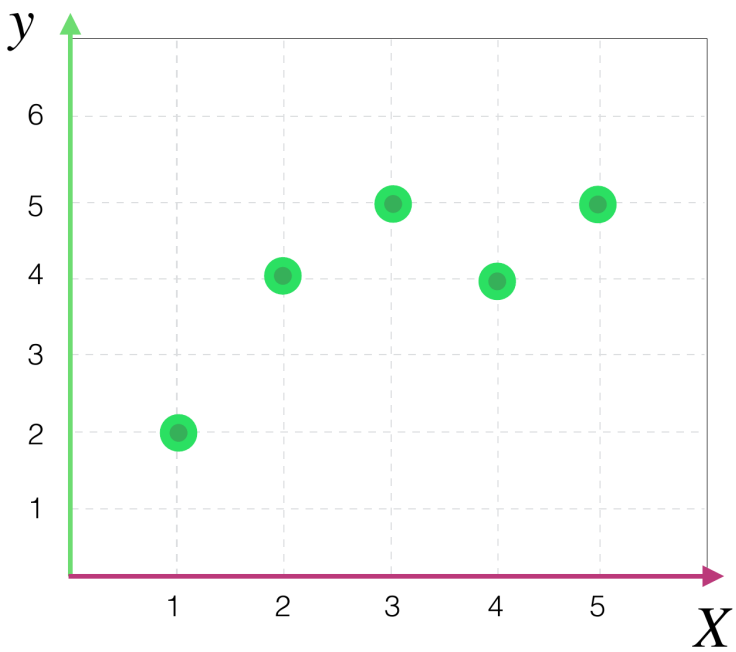


x	y
1	2
2	4
3	5
4	4
5	5

$\bar{x} = 3$

$\bar{y} = 4$

Principal Component Analysis



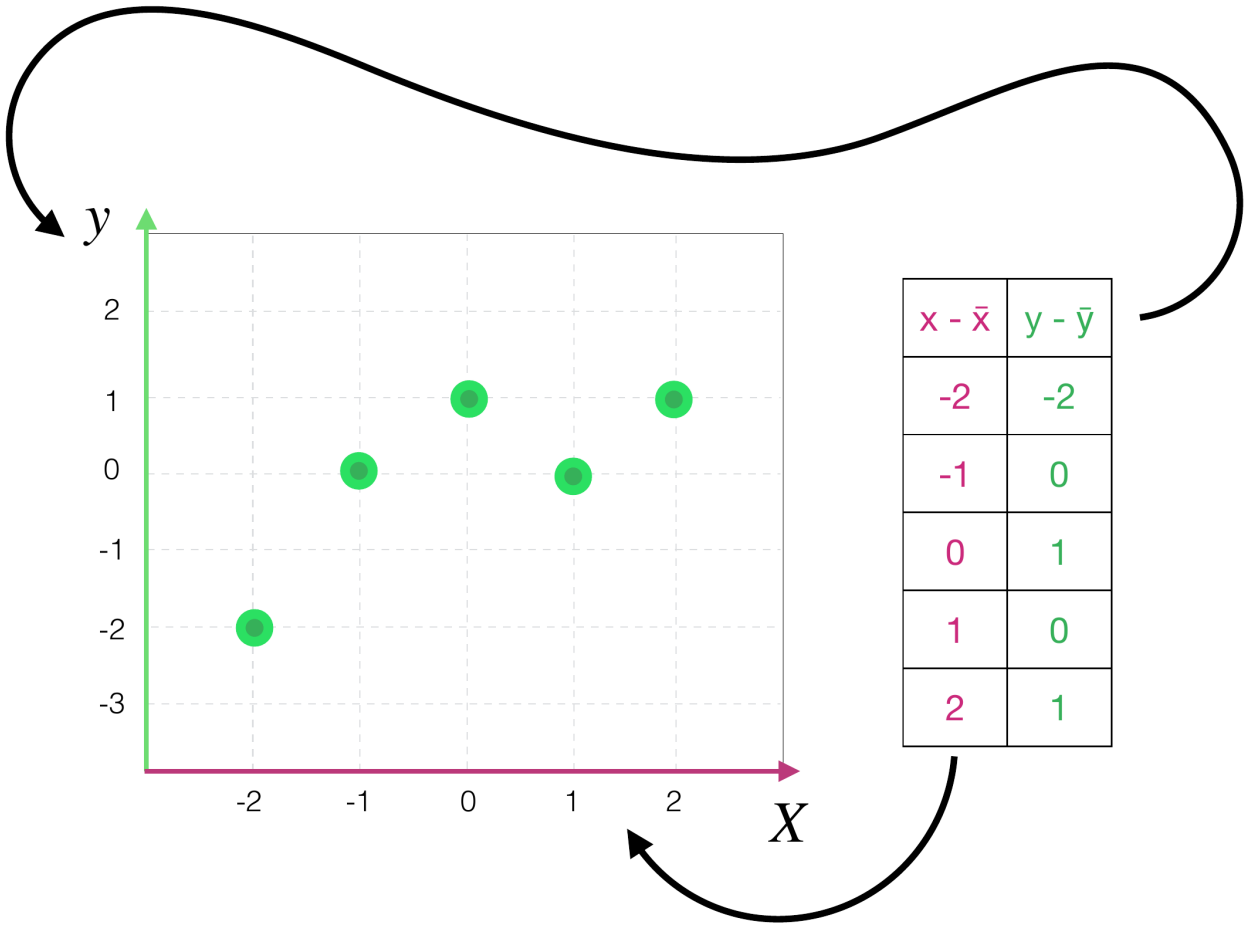
x	y
1	2
2	4
3	5
4	4
5	5

$\bar{x} = 3$

$\bar{y} = 4$

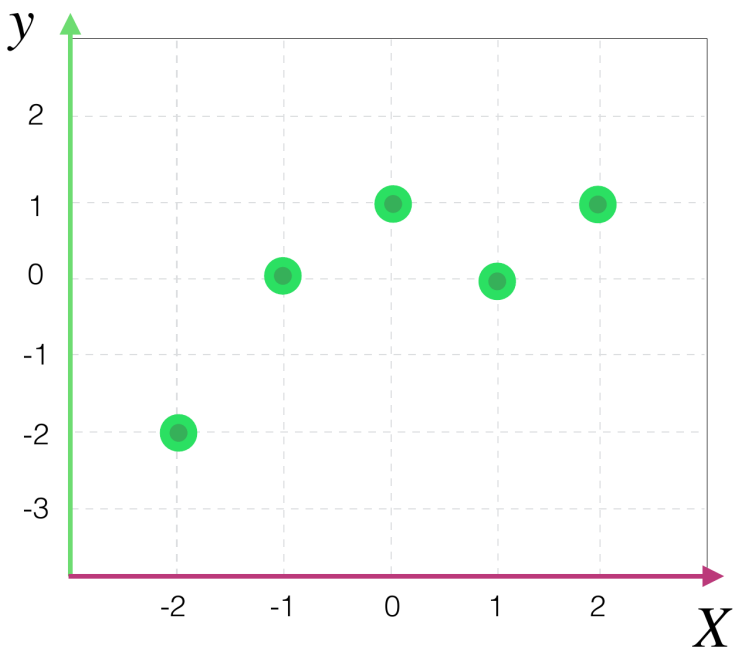
x - $\bar{x}$	y - $\bar{y}$
-2	-2
-1	0
0	1
1	0
2	1

Principal Component Analysis



x - x̄	y - ȳ
-2	-2
-1	0
0	1
1	0
2	1

Principal Component Analysis



Z

$x - \bar{x}$	$y - \bar{y}$
-2	-2
-1	0
0	1
1	0
2	1

Principal Component Analysis

Transpose the matrix of coordinates

Z

-2	-2
-1	0
0	1
1	0
2	1

Principal Component Analysis

Transpose the matrix of coordinates

Z

-2	-2
-1	0
0	1
1	0
2	1

What are the **dimensions** of the transposed matrix?

Principal Component Analysis

Transpose the matrix of coordinates

Z

-2	-2
-1	0
0	1
1	0
2	1

Z^T

Principal Component Analysis

Transpose the matrix of coordinates

Z

-2	-2
-1	0
0	1
1	0
2	1

Z^T

-2	-1	0	1	2
-2	0	1	0	1

Principal Component Analysis

$$Z^{\top} \times Z = S$$

Principal Component Analysis

Z^T

-2	-1	0	1	2
-2	0	1	0	1

$\times$

Z

-2	-2
-1	0
0	1
1	0
2	1

$=$

S

?	?
?	?

Principal Component Analysis

Z^T

-2	-1	0	1	2
-2	0	1	0	1

$\times$

Z

-2	-2
-1	0
0	1
1	0
2	1

$=$

S

10	6
6	6

Principal Component Analysis

Z^T

-2	-1	0	1	2
-2	0	1	0	1

$\times$

Z

-2	-2
-1	0
0	1
1	0
2	1

$=$

S

2.5	1.5
1.5	1.5

$\times 4$

Principal Component Analysis

Z^T

-2	-1	0	1	2
-2	0	1	0	1

$\times$

Z

-2	-2
-1	0
0	1
1	0
2	1

$=$

S

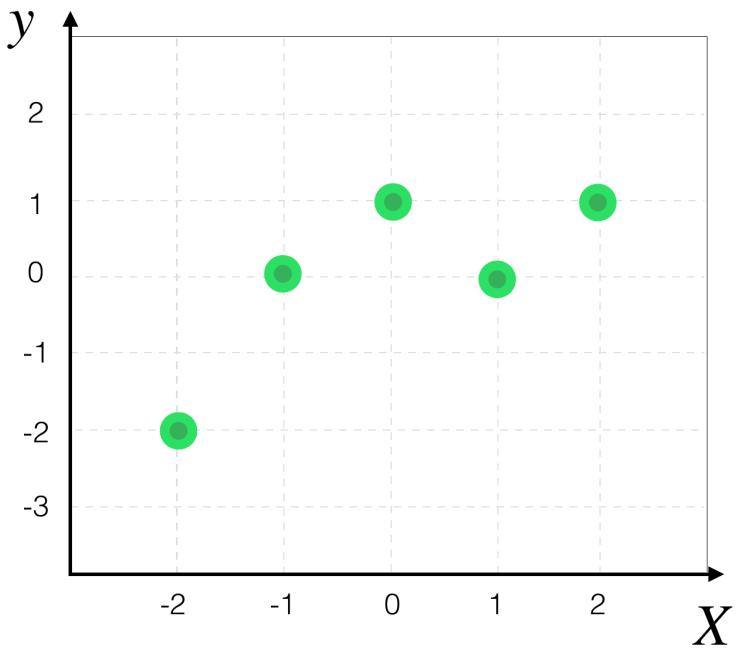
2.5	1.5
1.5	1.5

$\times 4$

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?



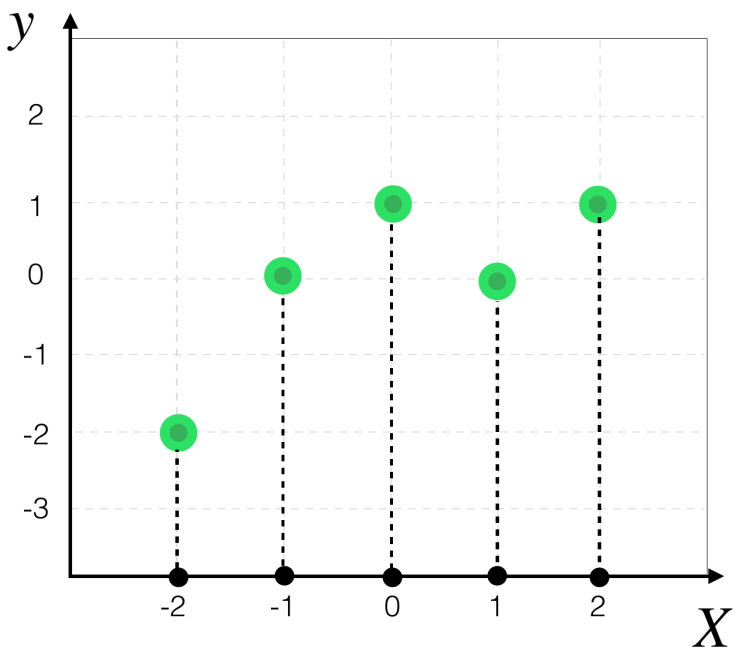
S

2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?



S

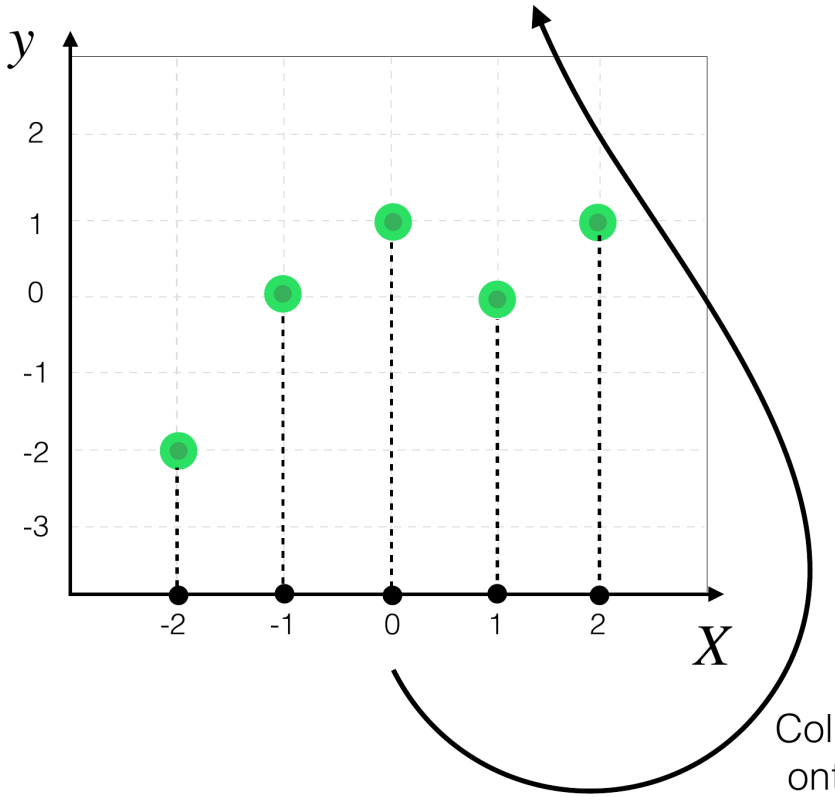
2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2]



Collect all projected onto **X axis** values

S

2.5	1.5
1.5	1.5

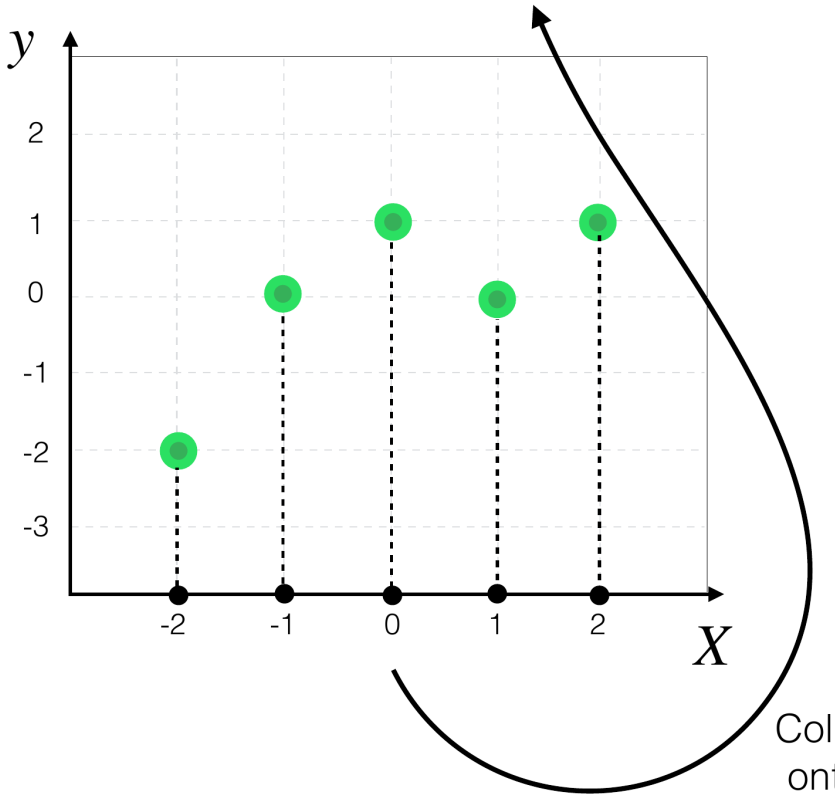
Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2]

mean([-2, -1, 0, 1, 2]) = ?



Collect all projected onto **X axis** values

S

2.5	1.5
1.5	1.5

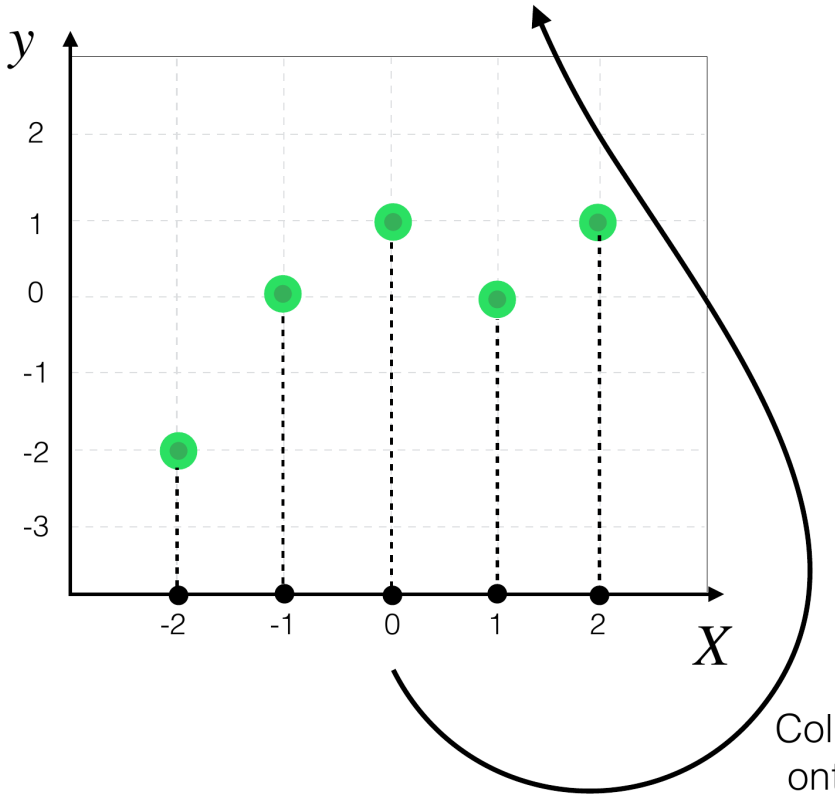
Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2]

mean([-2, -1, 0, 1, 2]) = 0



S

2.5	1.5
1.5	1.5

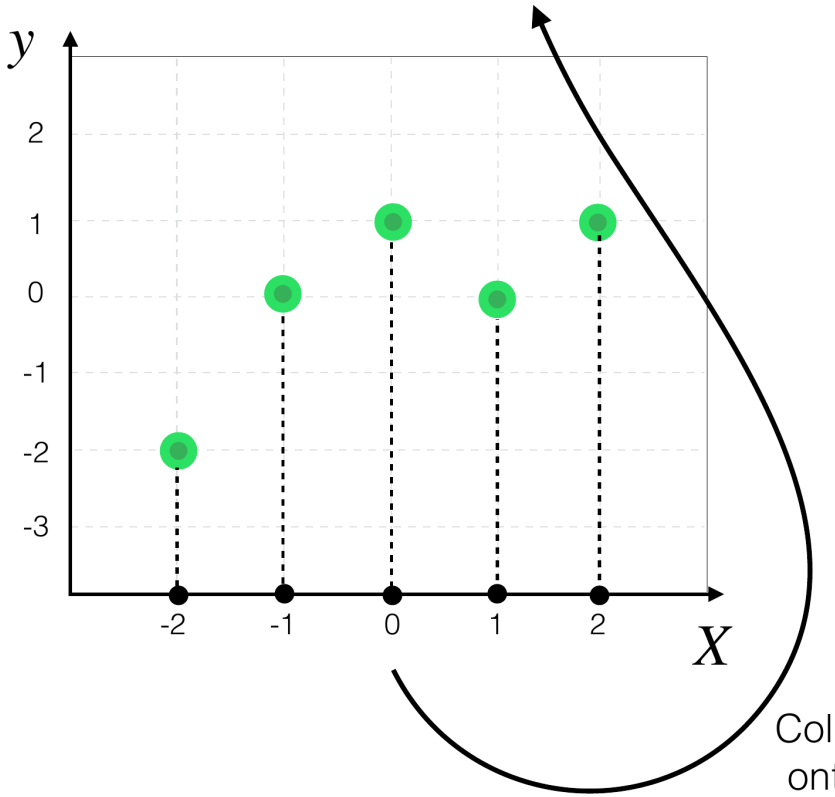
Covariance matrix

Collect all projected onto **X axis** values

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] $\bar{\mathbf{x}} = 0$



Collect all projected onto **X axis** values

S

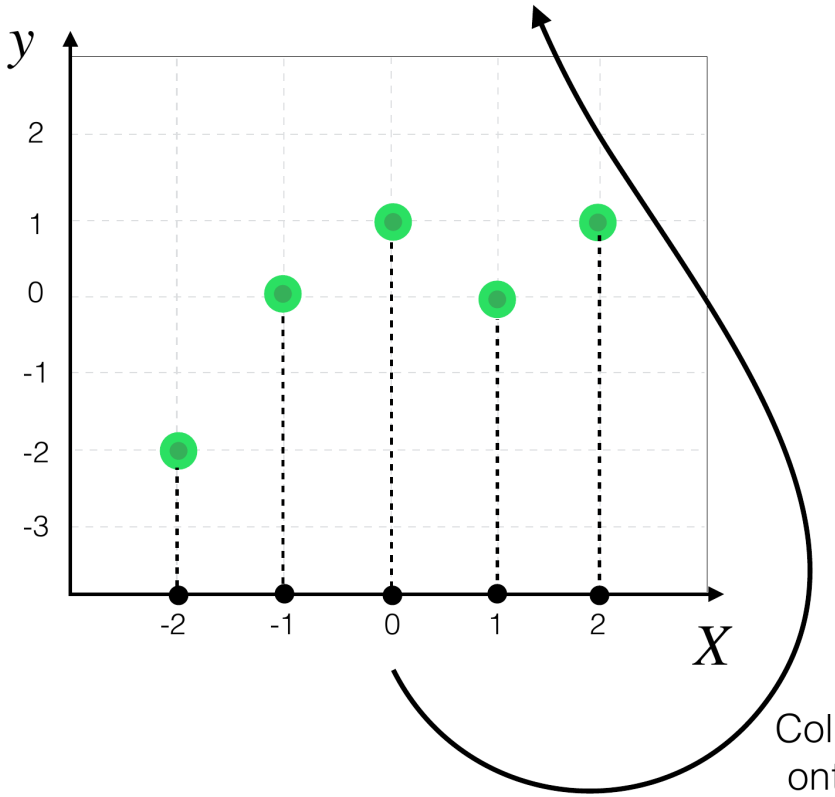
2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] $\quad \bar{\mathbf{x}} = 0 \quad \sigma = \dfrac{\sum (x_i - \bar{x})^2}{n-1}$



Collect all projected onto **X axis** values

S

2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] $\bar{x} = 0$

$$\sigma = \frac{\sum (x_i - \bar{x})^2}{n - 1}$$

S

Covariance matrix

Collect all projected
onto **X axis** values

Principal Component Analysis

Variance $\longrightarrow \sigma = \dfrac{\sum (x_i - \bar{x})^2}{n-1}$

Covariance matrix

Principal Component Analysis

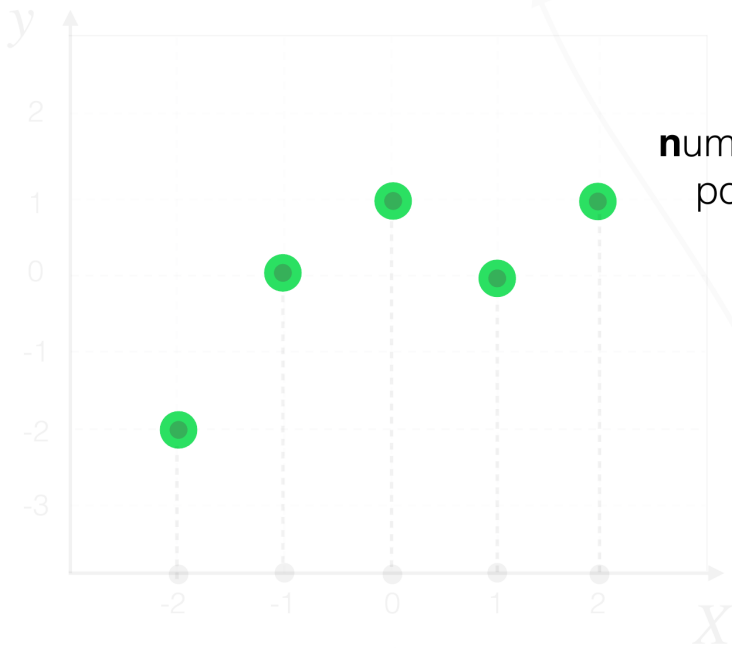
Variance $\longrightarrow \sigma = \dfrac{\sum (x_i - \bar{x})^2}{n - 1}$

number of points

Principal Component Analysis

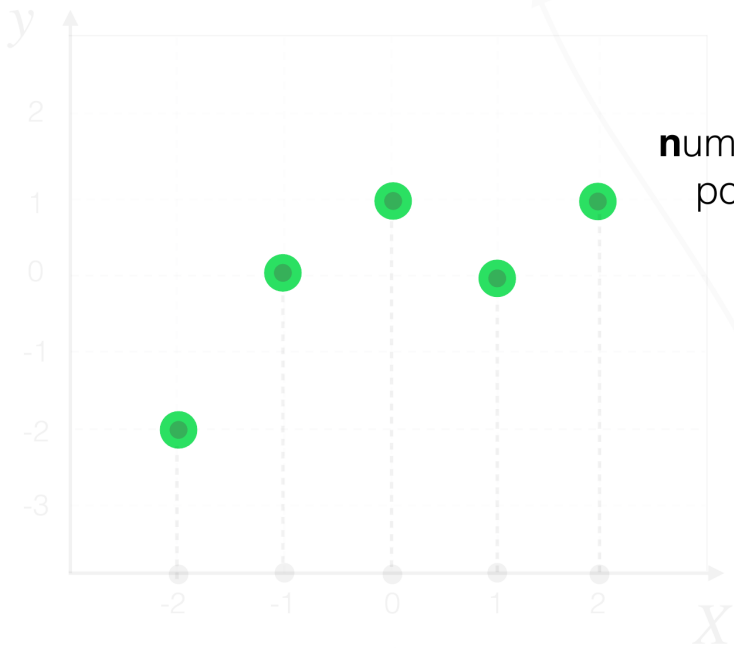
Variance $\longrightarrow \sigma = \dfrac{\sum (x_i - \bar{x})^2}{5 - 1}$

number of points



Principal Component Analysis

Variance $\longrightarrow \sigma = \dfrac{\sum (x_i - \bar{x})^2}{4}$



number of points

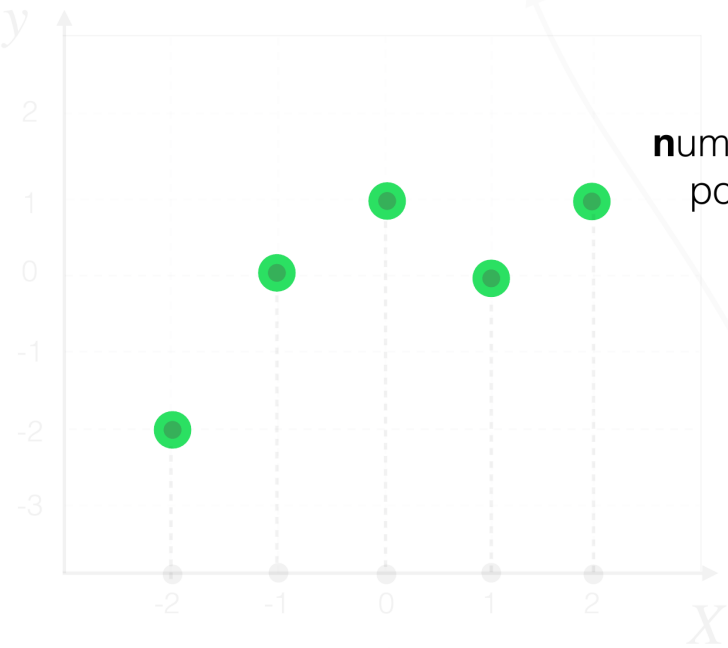
Principal Component Analysis

mean of all points

$$\textbf{Variance} \longrightarrow \sigma = \frac{\sum (x_i - \bar{x})^2}{4}$$

$\bar{\mathbf{x}} = 0$

number of points



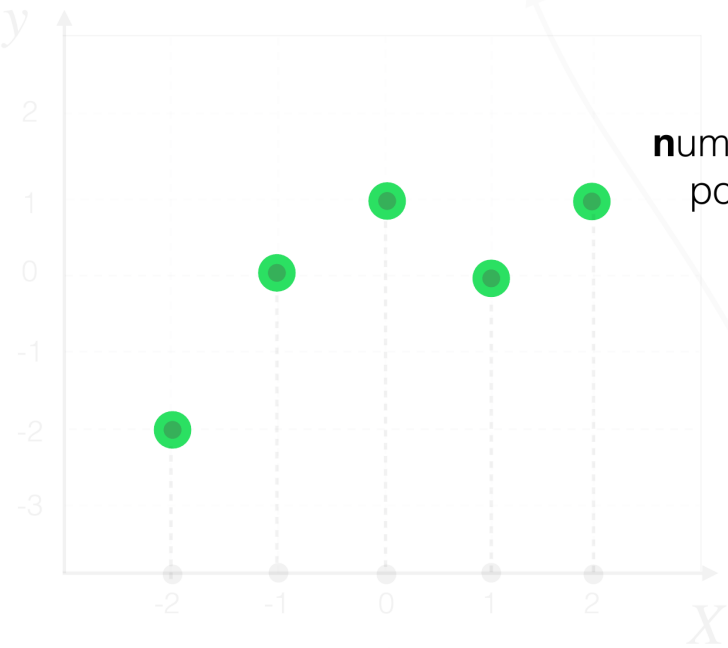
Covariance matrix

Principal Component Analysis

mean of all points

$$\textbf{Variance} \longrightarrow \sigma = \frac{\sum (x_i - 0)^2}{4} \qquad \bar{\mathbf{x}} = 0$$

number of points

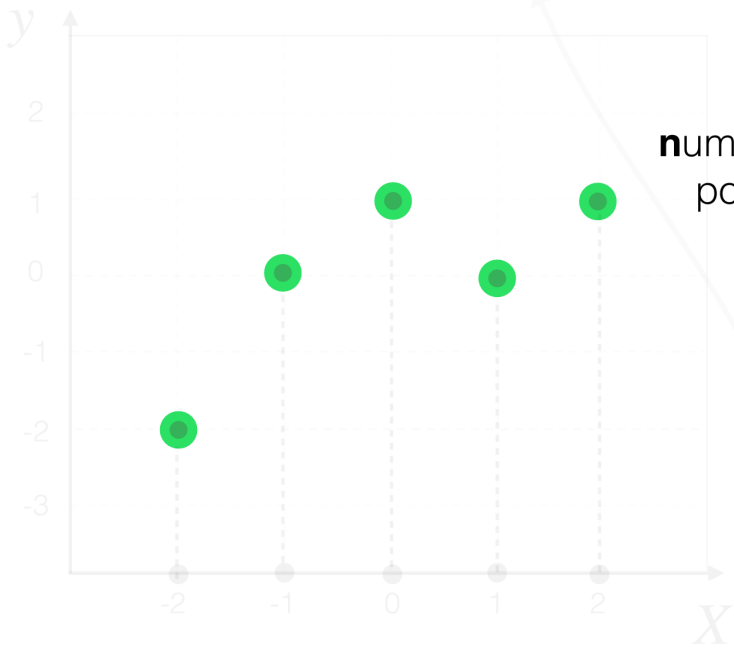


Covariance matrix

Principal Component Analysis

$\bar{\mathbf{x}} = 0$ **m**ean of all points

$$\textbf{Variance} \longrightarrow \sigma = \frac{\sum (x_i)^2}{4}$$



number of points

Covariance matrix

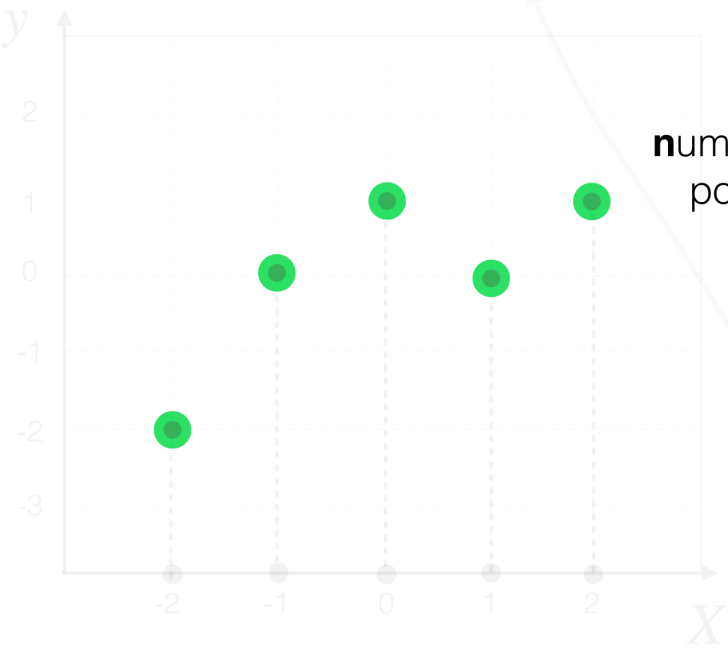
Principal Component Analysis

value of each point

$\bar{\mathbf{x}} = 0$ **m**ean of all points

$$\textbf{Variance} \longrightarrow \sigma = \frac{\sum (x_i)^2}{4}$$

number of points



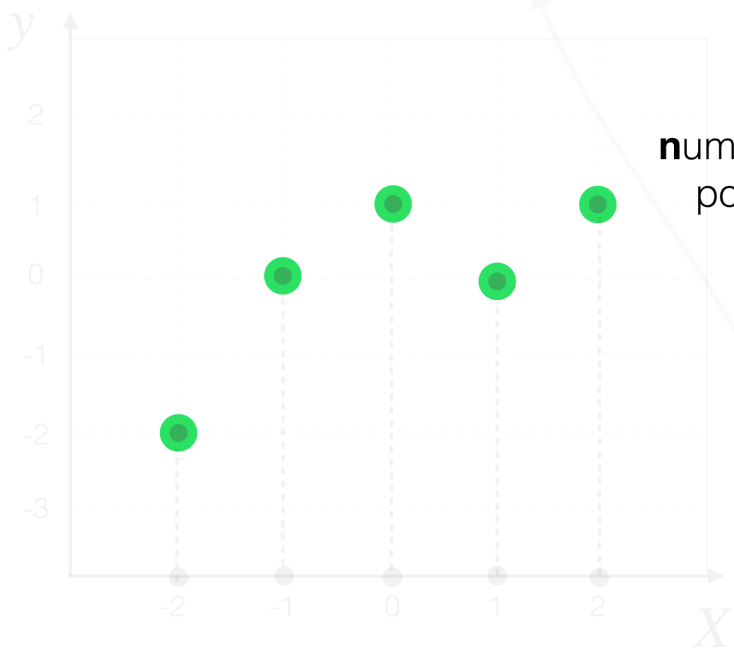
Covariance matrix

Principal Component Analysis

[-2, -1, 0, 1, 2] **value** of each point

$\bar{\mathbf{x}} = 0$ **m**ean of all points

Variance $\longrightarrow \sigma = \dfrac{\sum (x_i)^2}{4}$



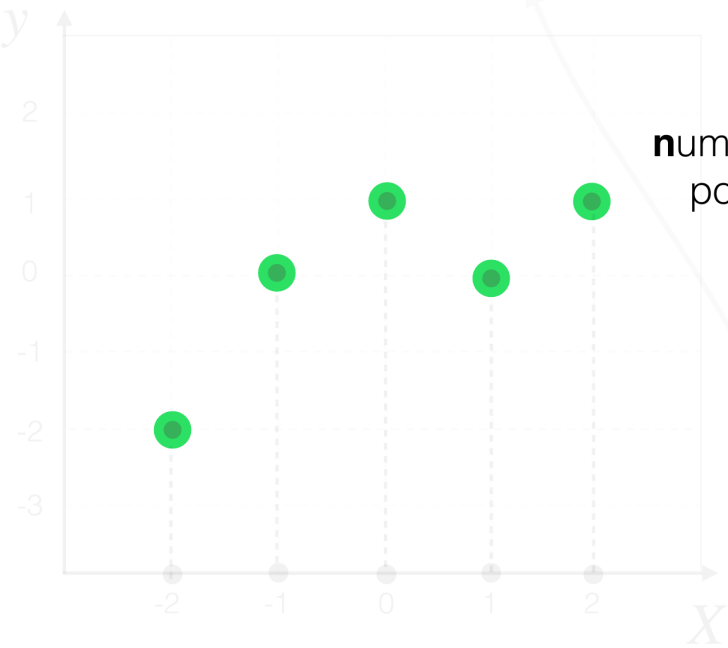
number of points

Covariance matrix

Principal Component Analysis

[-2, -1, 0, 1, 2] **value** of each point → $\bar{\mathbf{x}} = 0$ **m**ean of all points

Variance → $\sigma = \frac{(-2)^2 + (-1)^2 + (0)^2 + (1)^2 + (2)^2}{4}$



number of points

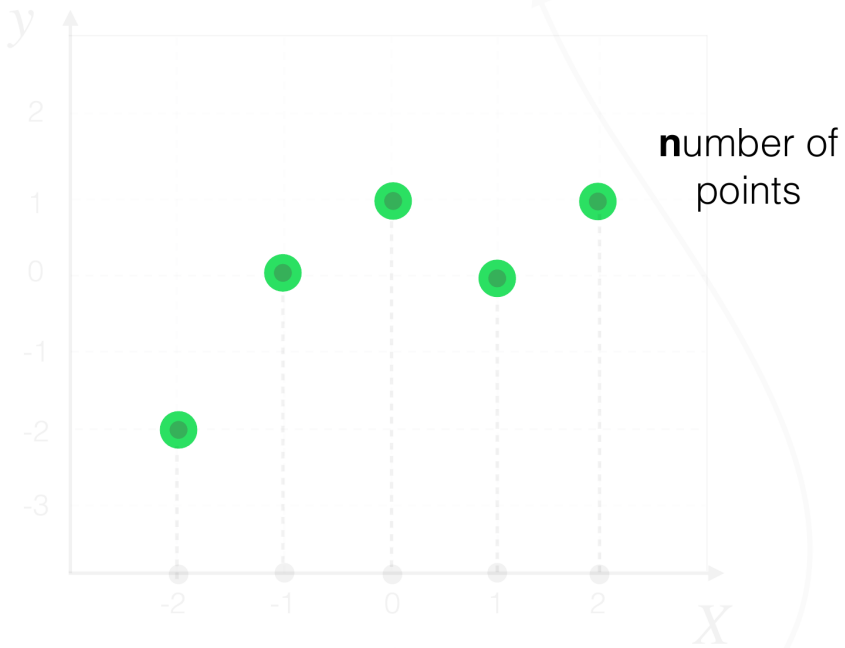
Covariance matrix

Principal Component Analysis

[-2, -1, 0, 1, 2] **value** of each point

$\bar{\mathbf{x}} = 0$ **m**ean of all points

$$\textbf{Variance} \longrightarrow \sigma = \frac{10}{4}$$



number of points

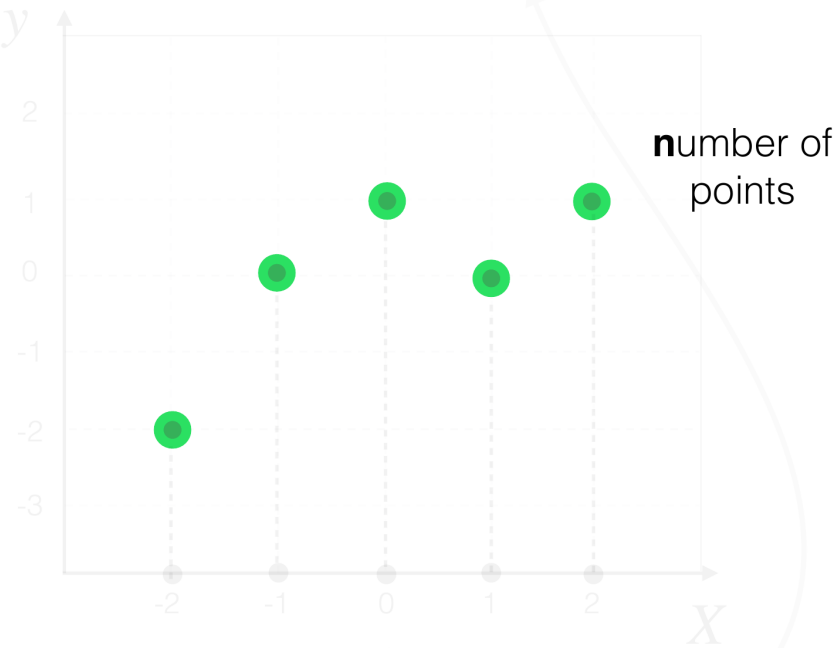
Covariance matrix

Principal Component Analysis

[-2, -1, 0, 1, 2] **value** of each point

$\bar{\mathbf{x}} = 0$ **m**ean of all points

Variance $\longrightarrow \sigma = 2.5$



number of points

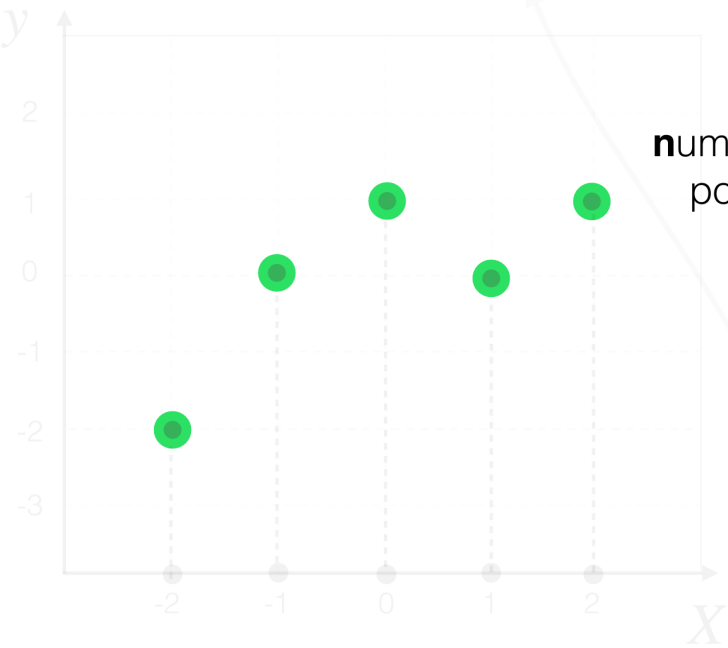
Covariance matrix

Principal Component Analysis

[-2, -1, 0, 1, 2] **value** of each point

$\bar{\mathbf{x}} = 0$ **m**ean of all points

Variance $\longrightarrow \sigma = 2.5$



number of points

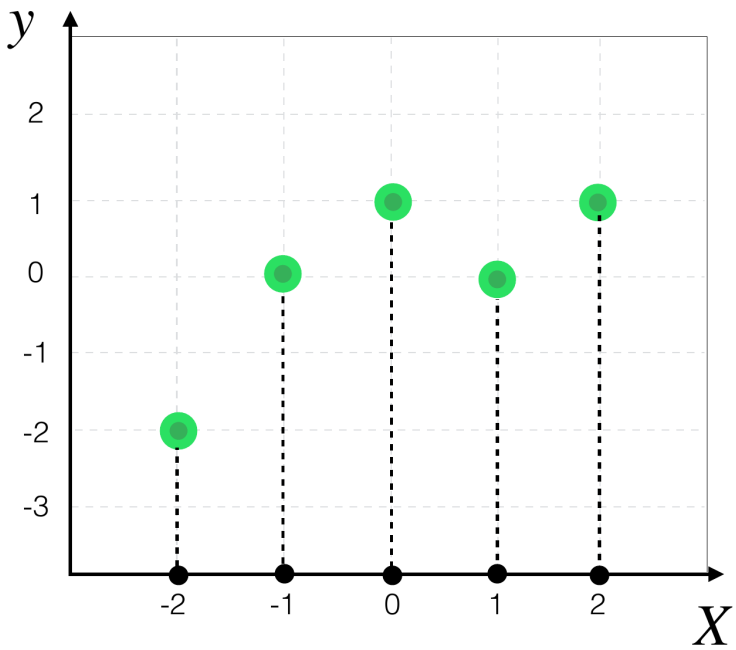
$$\sigma = \frac{\sum (x_i - \bar{x})^2}{n - 1}$$

Variance is an expected value of the squared deviation from the mean

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] $\bar{\mathbf{x}} = 0$ $\sigma = 2.5$



S

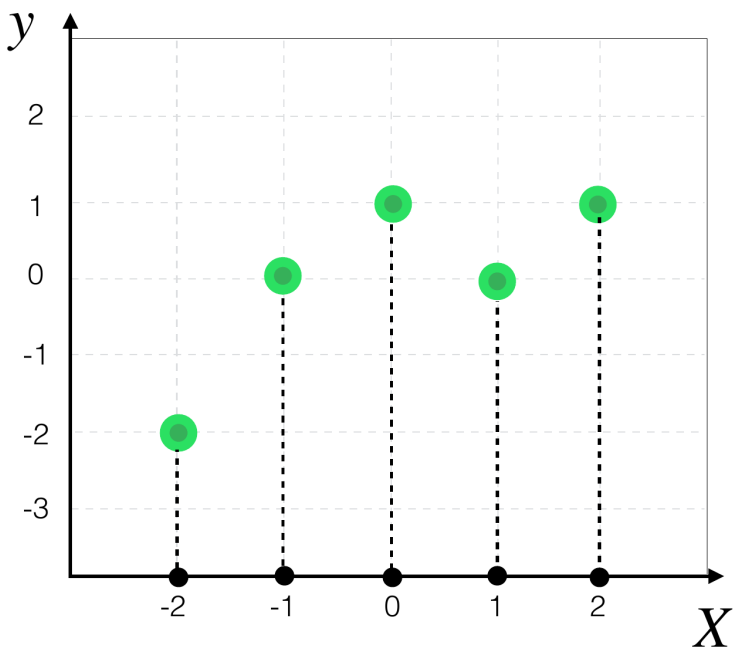
2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] $\bar{\mathbf{x}} = 0$ $\sigma = 2.5$



Variance along **first** axis

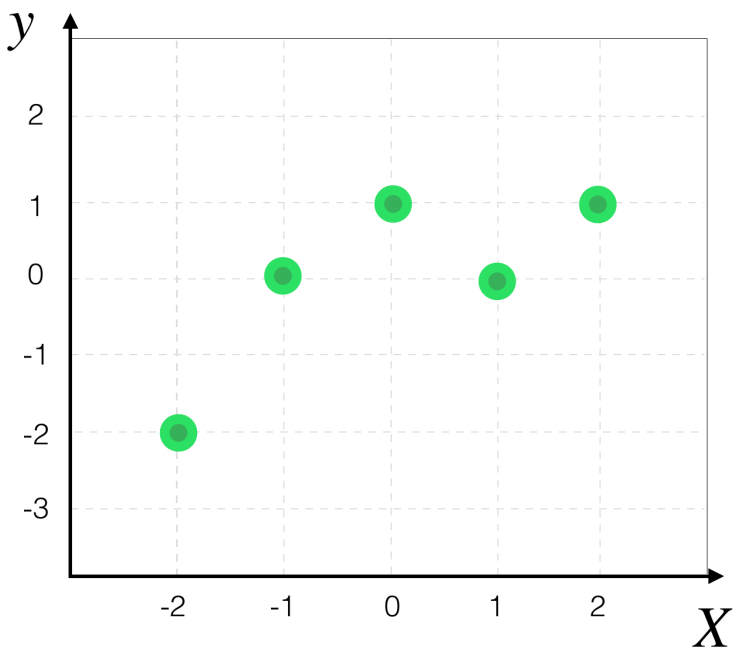
S

2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?



Variance along **first** axis

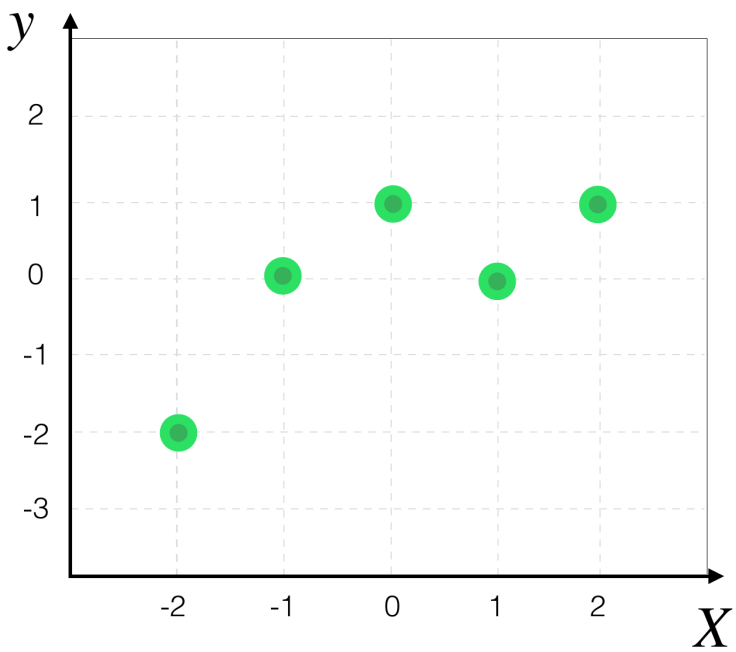
S

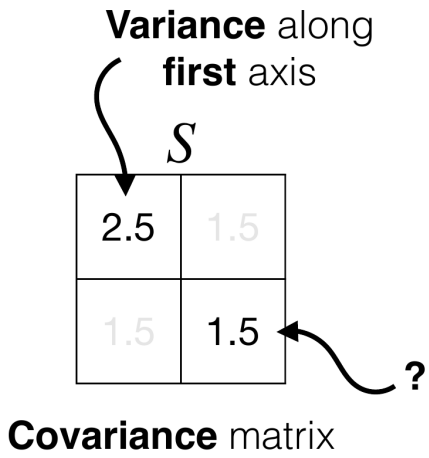
2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

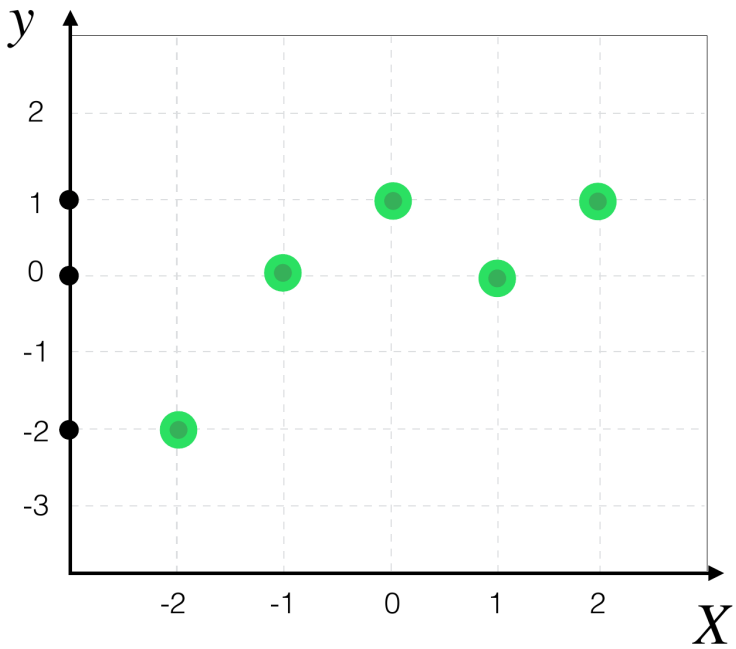
How to **interpret** values in **covariance** matrix?





Principal Component Analysis

How to **interpret** values in **covariance** matrix?



Variance along **first** axis

S

2.5	1.5
1.5	1.5

Variance along **second** axis

Covariance matrix

Principal Component Analysis

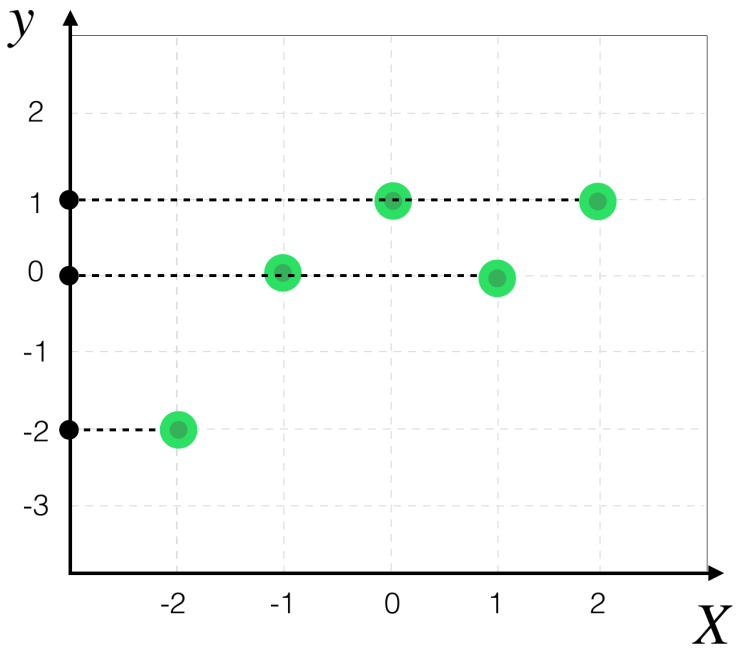
How to **interpret** values in **covariance** matrix?

value of each point

number of points

mean of all points

$$\sigma = \frac{\sum (y_i - \bar{y})^2}{n - 1}$$



Variance along **first** axis

S

2.5	1.5
1.5	1.5

Variance along **second** axis

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

value of each point

[-2, 0, 0, 1, 1]

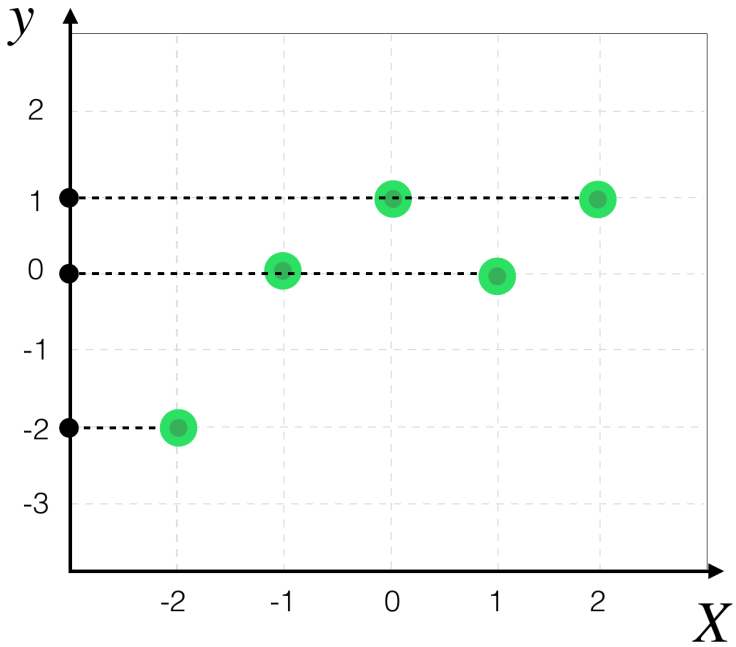
number of points

5

mean of all points

$\bar{\mathbf{y}} = 0$

$$\sigma = \frac{\sum (y_i - \bar{y})^2}{n - 1}$$



Variance along **first** axis

S

2.5	1.5
1.5	1.5

Variance along **second** axis

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

value of each point

[-2, 0, 0, 1, 1]

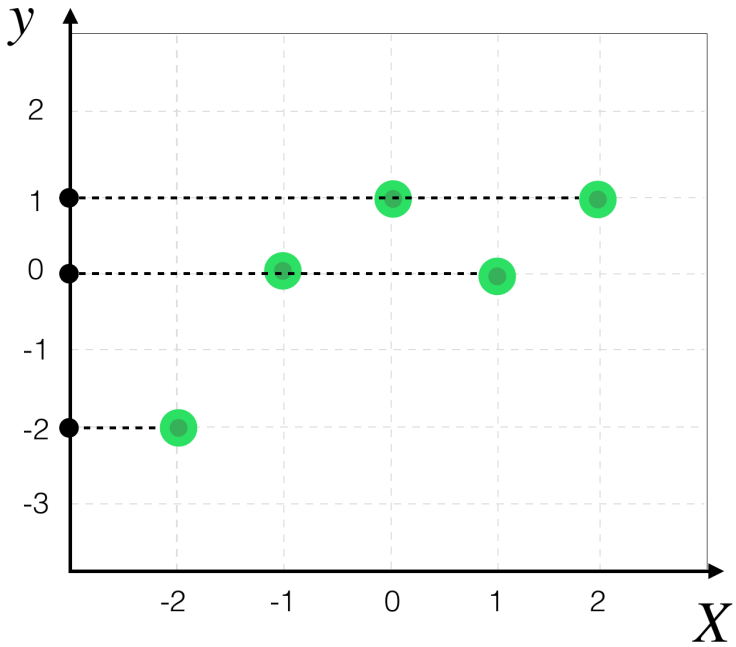
number of points

5

mean of all points

$\bar{\mathbf{y}} = 0$

$$\sigma = \frac{6}{4}$$



Variance along **first** axis

S

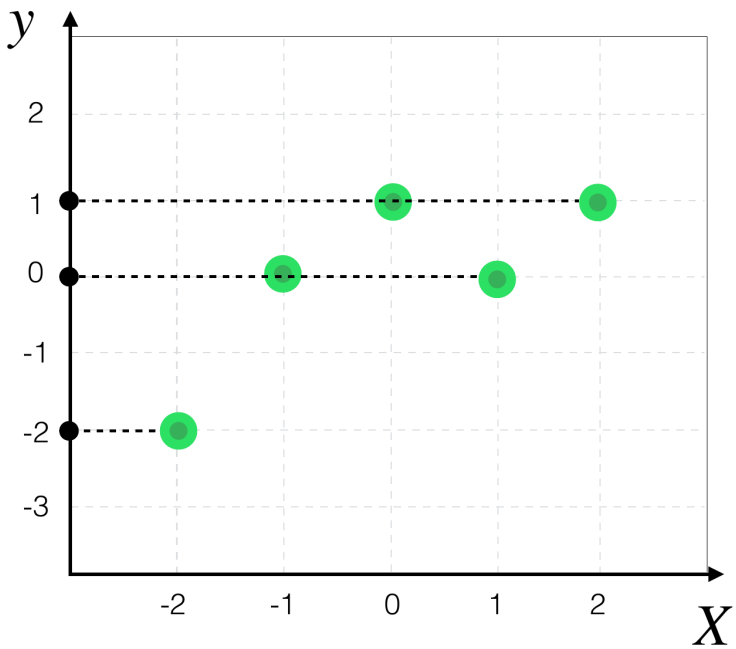
2.5	1.5
1.5	1.5

Variance along **second** axis

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?



Variance along **first** axis

S

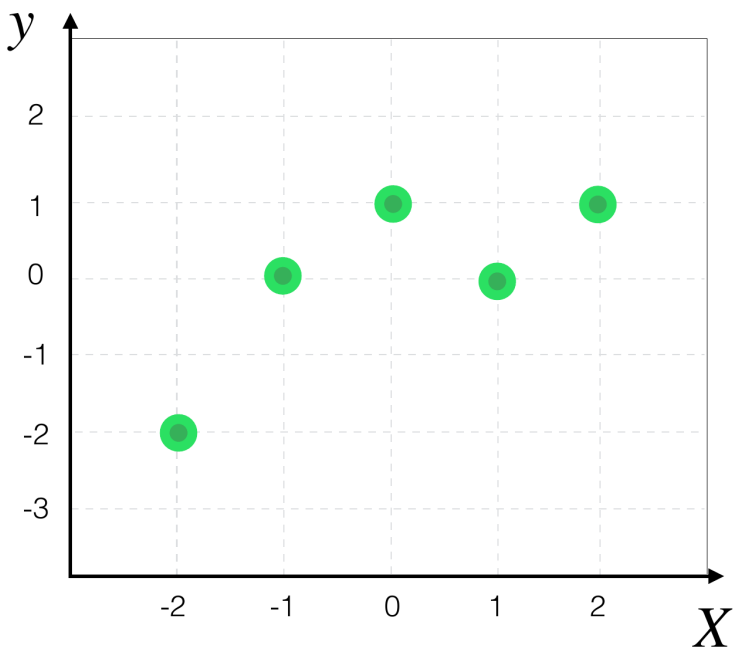
2.5	1.5
1.5	1.5

Variance along **second** axis

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?



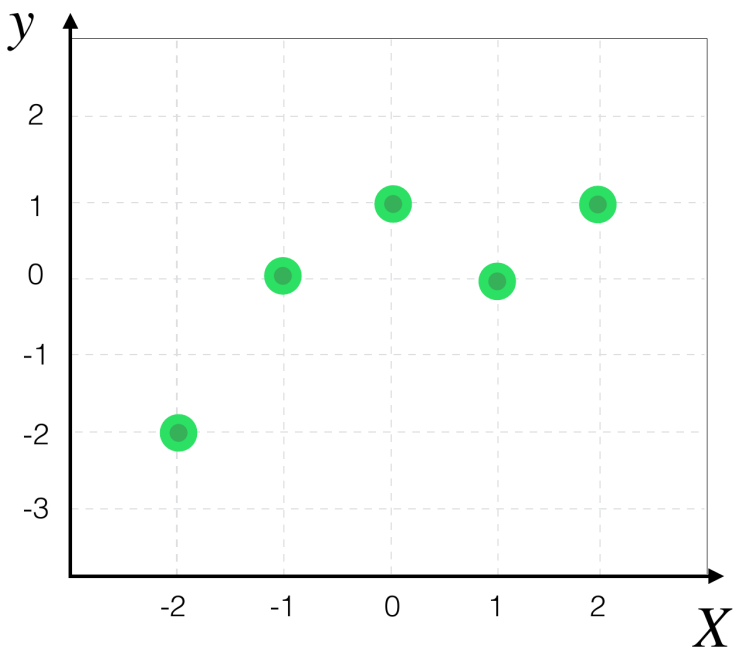
S

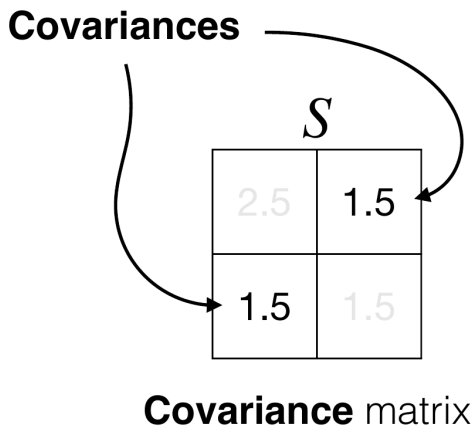
2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

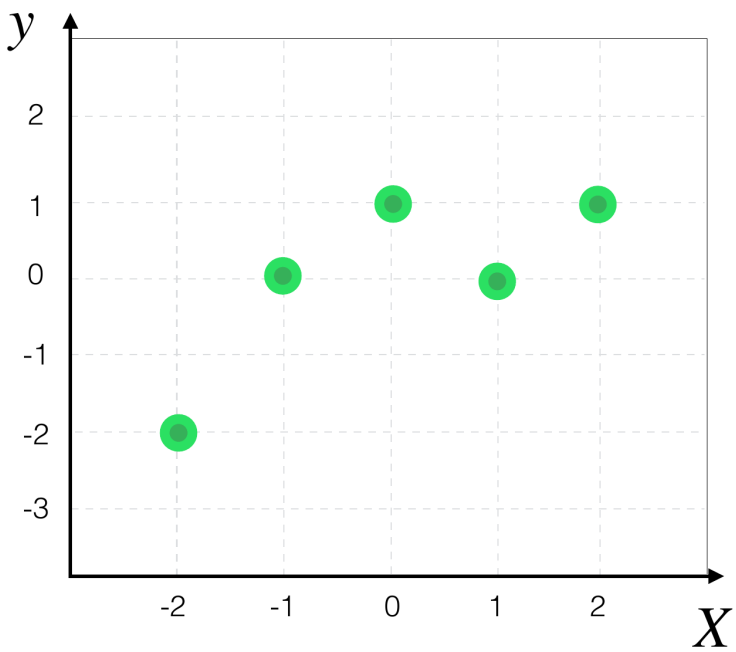


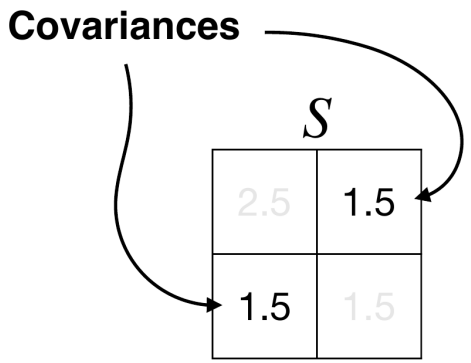


Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

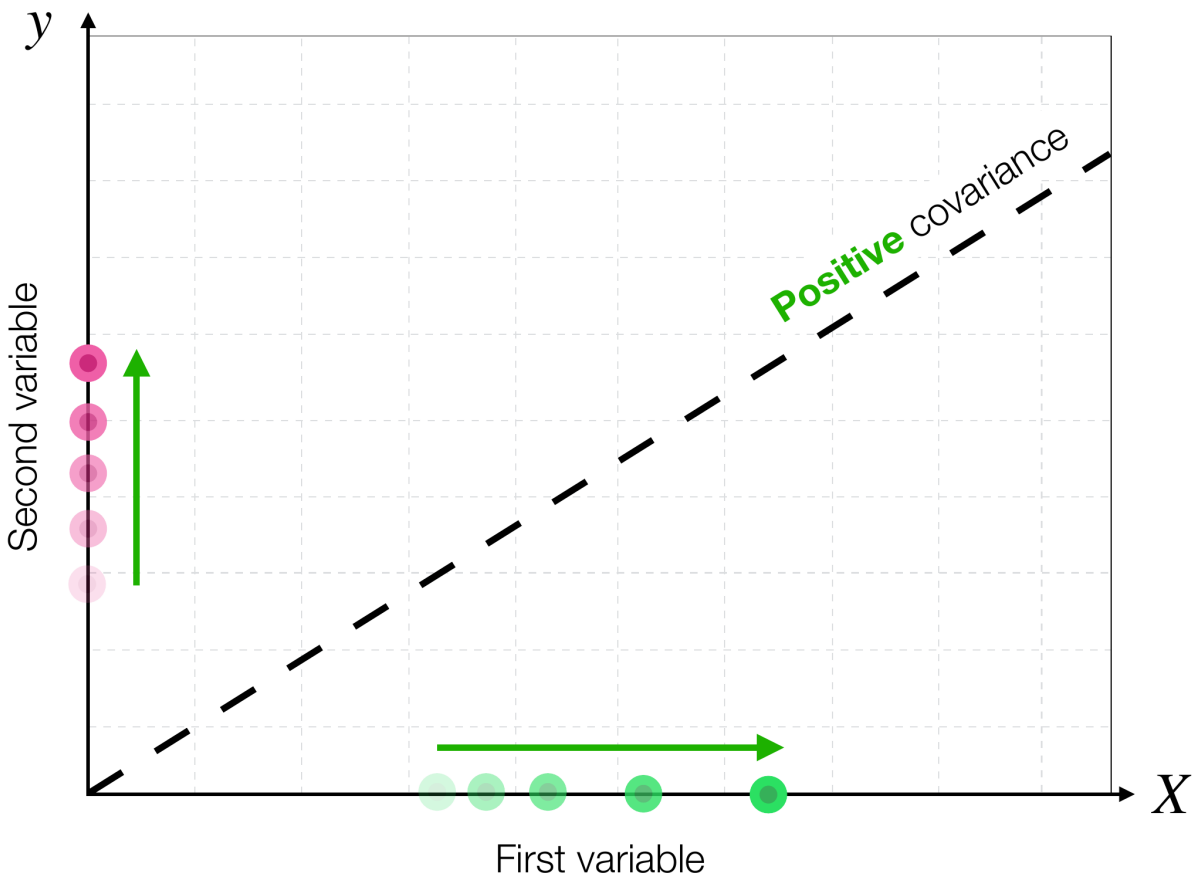




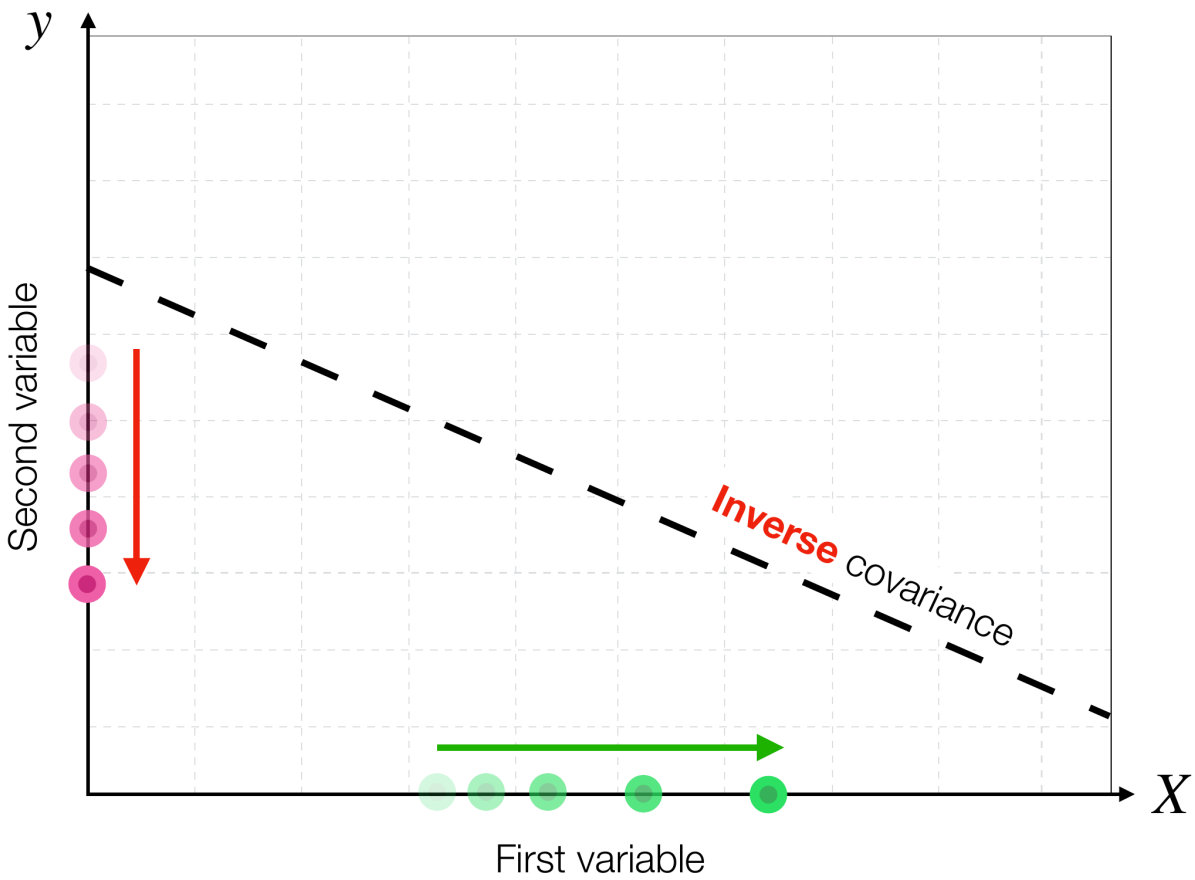
Covariance matrix

Covariance indicates how two variables are related. A **positive** covariance means the variables are **positively related**, while a **negative** covariance means the variables are **inversely related**.

Principal Component Analysis

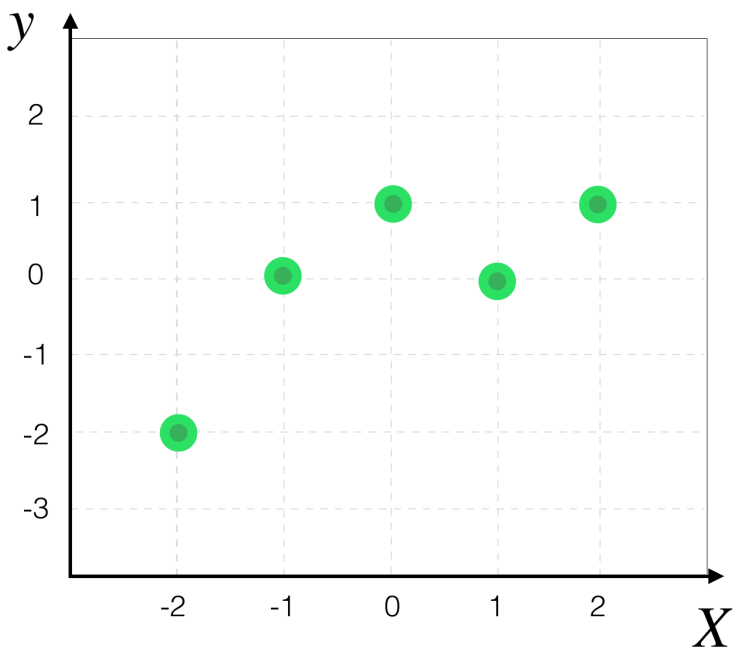


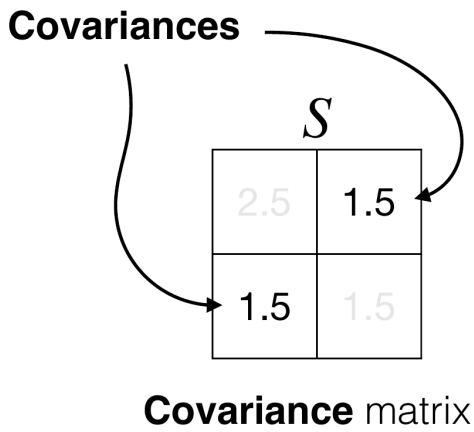
Principal Component Analysis



Principal Component Analysis

How to **interpret** values in **covariance** matrix?





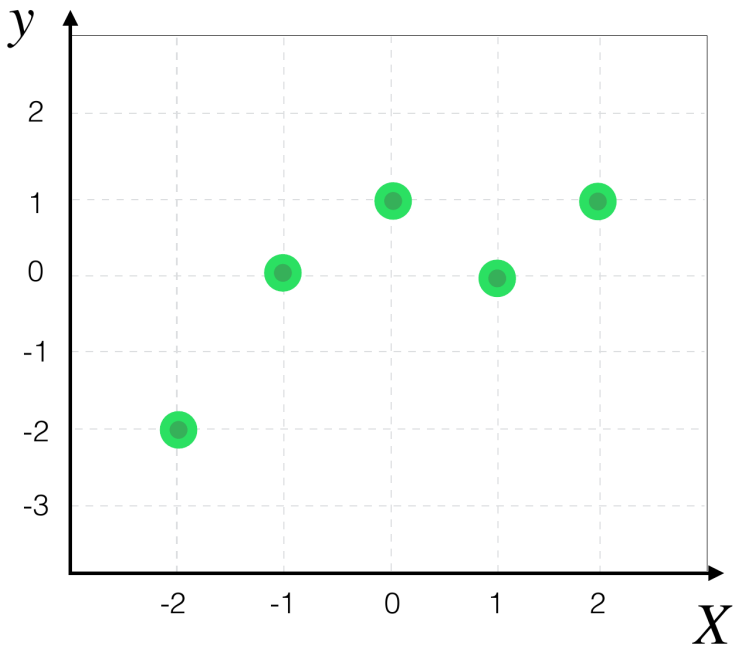
Covariance matrix

Principal Component Analysis

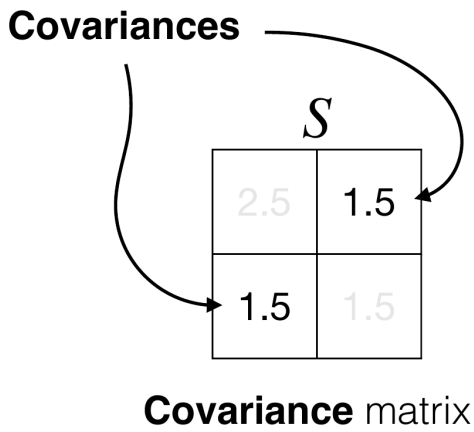
How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [-2, 0, 0, 1, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$



$$cov(x, y) = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n - 1}$$



Covariance matrix

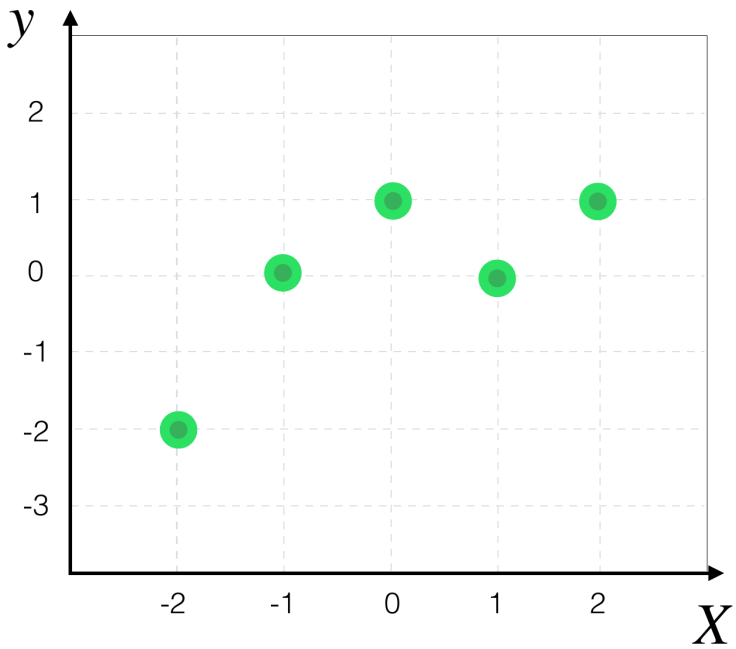
Principal Component Analysis

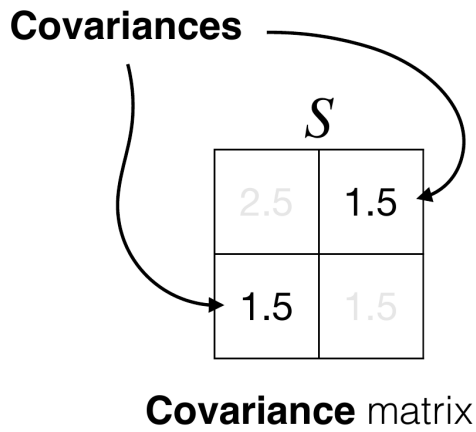
How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [-2, 0, 0, 1, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$

$$cov(x, y) = \frac{6}{4}$$





Covariance matrix

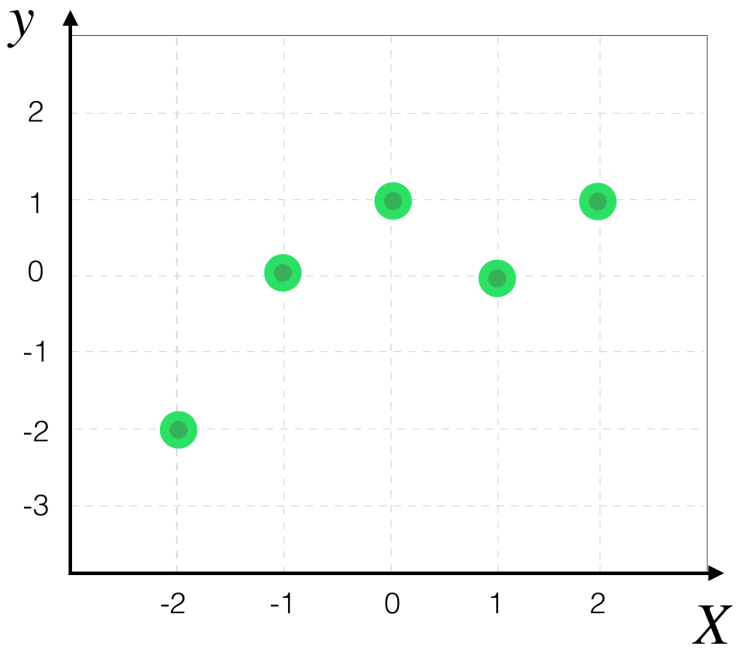
Principal Component Analysis

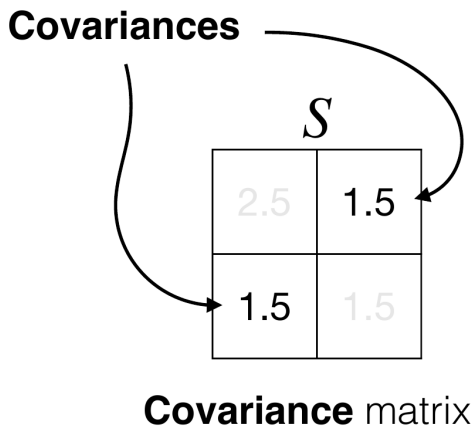
How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [-2, 0, 0, 1, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$

$$cov(x, y) = 1.5$$

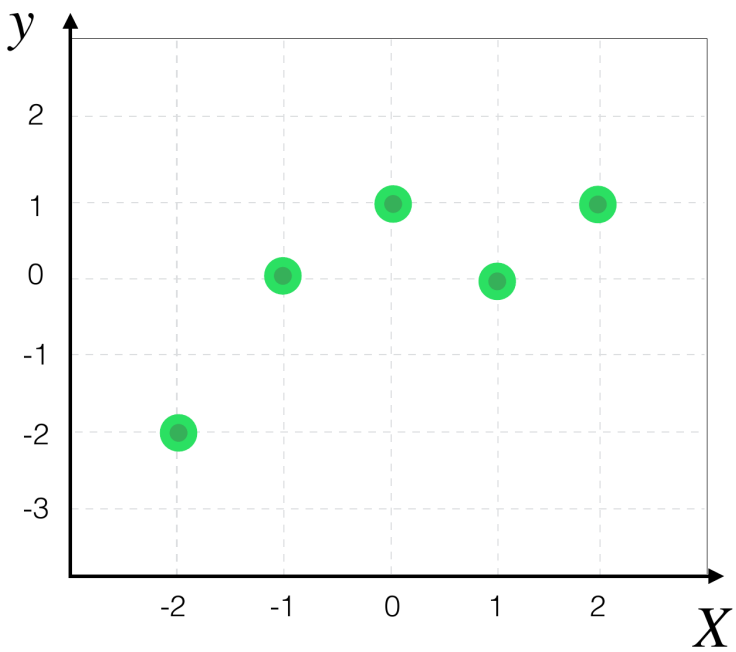




Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?



S

2.5	1.5
1.5	1.5

Covariance matrix

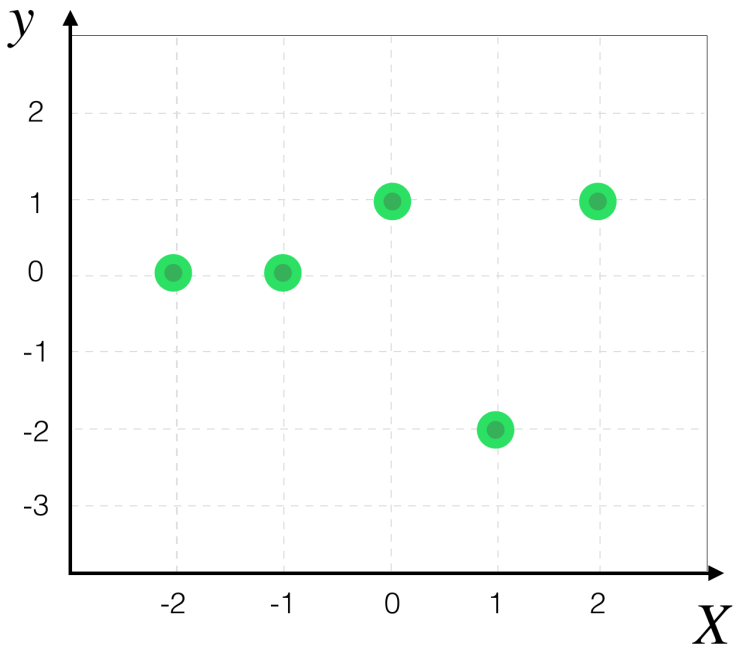
Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [0, 0, 1,-2, 1]

$\bar{\mathbf{x}} = ?$ $\bar{\mathbf{y}} = ?$

$$cov(x, y) = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n - 1}$$



S

2.5	?
?	1.5

Covariance matrix

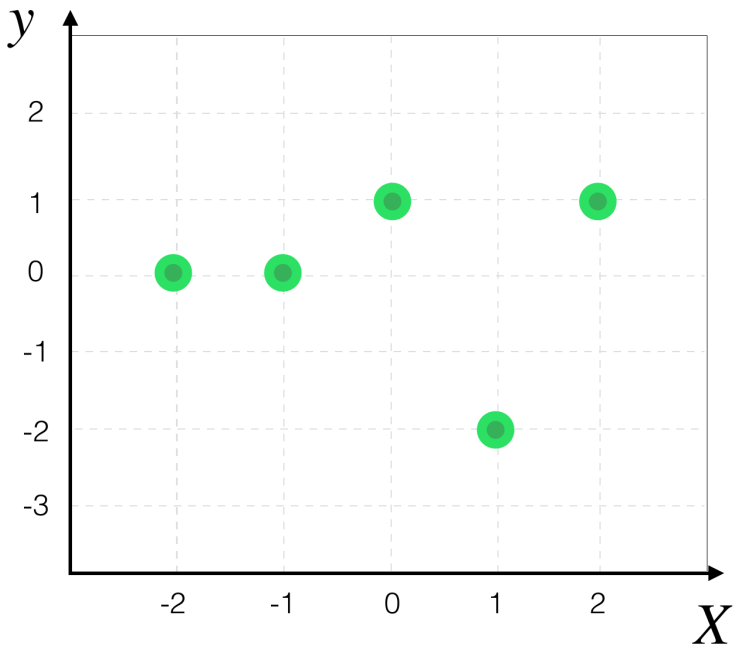
Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [0, 0, 1,-2, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$

$$cov(x, y) = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n - 1}$$



S

2.5	?
?	1.5

Covariance matrix

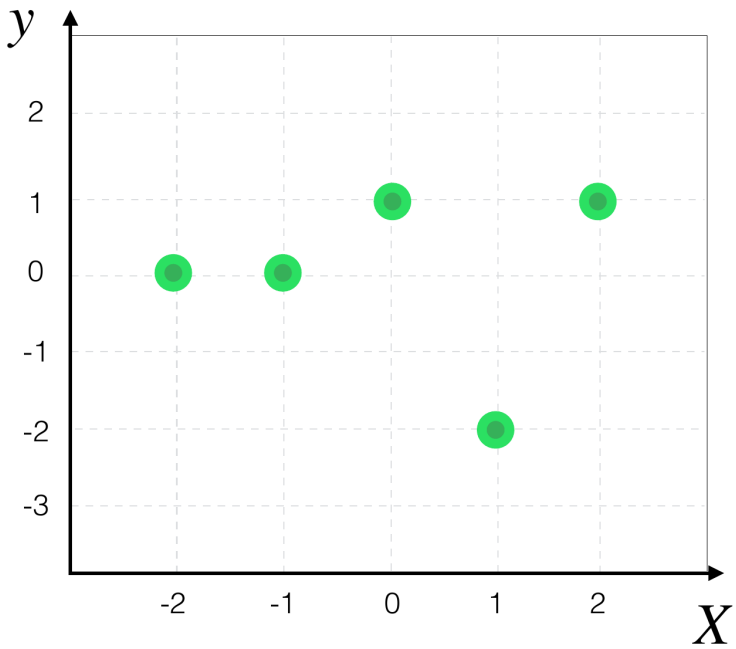
Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [0, 0, 1,-2, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$

$$cov(x, y) = \frac{\sum (x_i)(y_i)}{4}$$



S

2.5	?
?	1.5

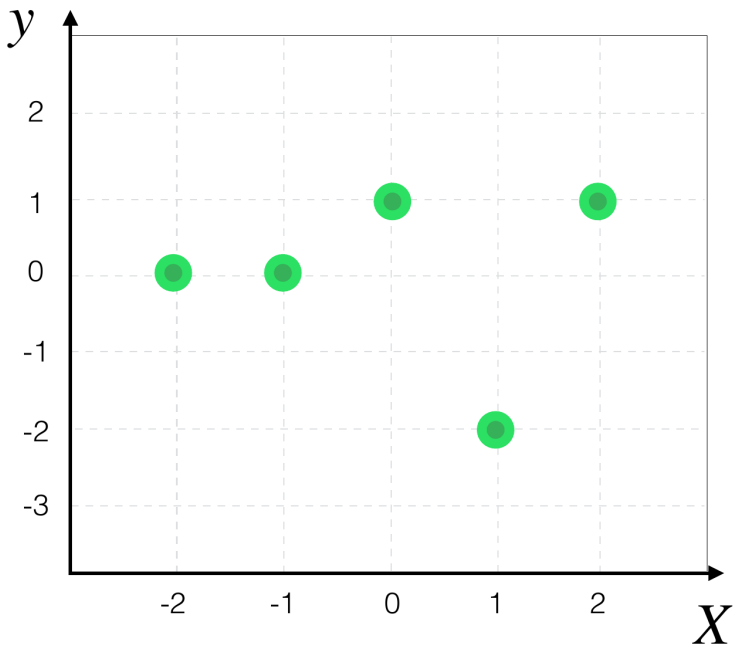
Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [0, 0, 1,-2, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$



$$cov(x, y) = \frac{(-2)(0) + (-1)(0) + (0)(1) + (1)(-2) + (2)(1)}{4}$$

S

2.5	?
?	1.5

Covariance matrix

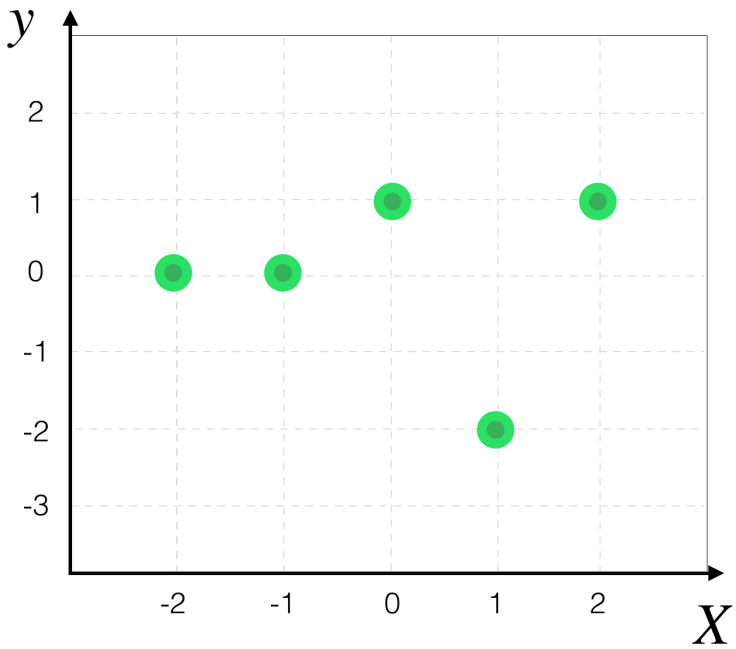
Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [0, 0, 1,-2, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$

$$cov(x, y) = \frac{0}{4} = 0$$



$$S$$

2.5	?
?	1.5

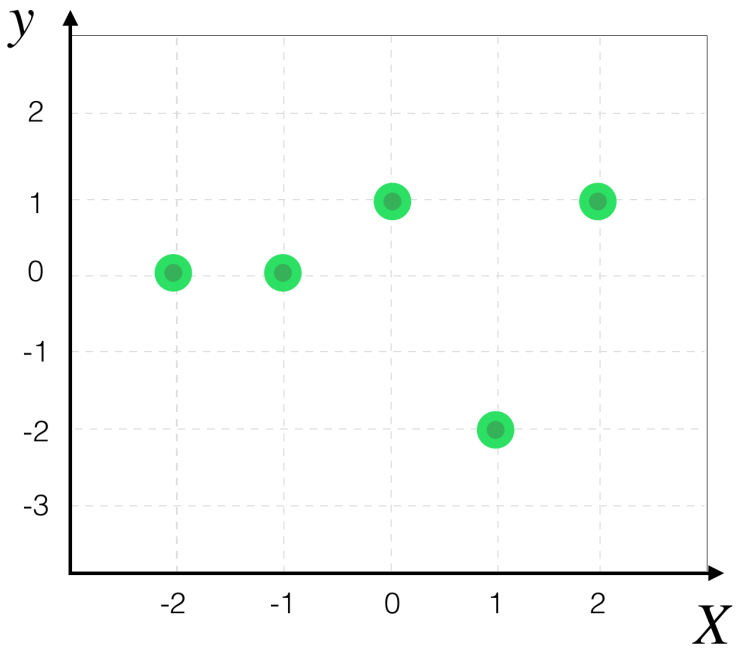
Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [0, 0, 1,-2, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$



$$cov(x, y) = \frac{0}{4} = 0$$

S

2.5	0
0	1.5

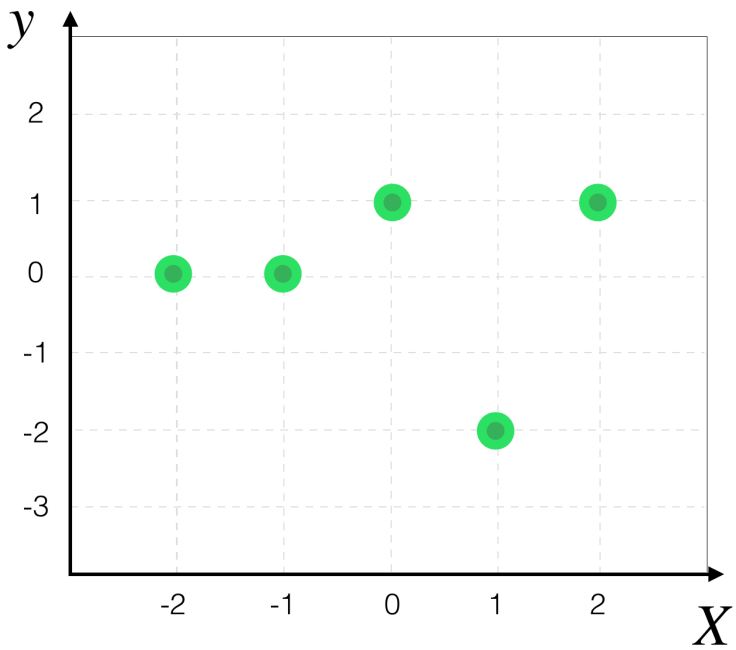
Covariance matrix

Principal Component Analysis

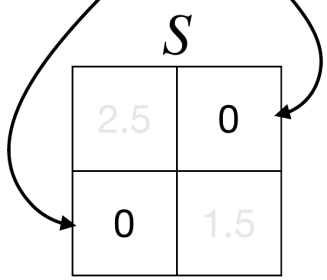
How to **interpret** values in **covariance** matrix?

[-2, -1, 0, 1, 2] [0, 0, 1,-2, 1]

$\bar{\mathbf{x}} = 0$ $\bar{\mathbf{y}} = 0$



$$cov(x, y) = \frac{0}{4} = 0$$

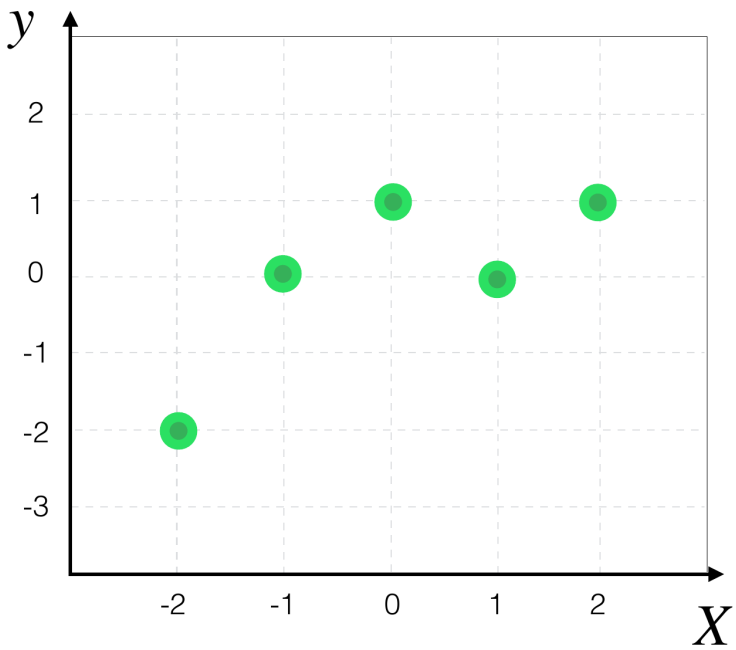


Covariance matrix

Covariance **0** means that there is **no relationship** between two variables. Knowing something about the value of one does not say anything about the value of the other.

Principal Component Analysis

How to **interpret** values in **covariance** matrix?



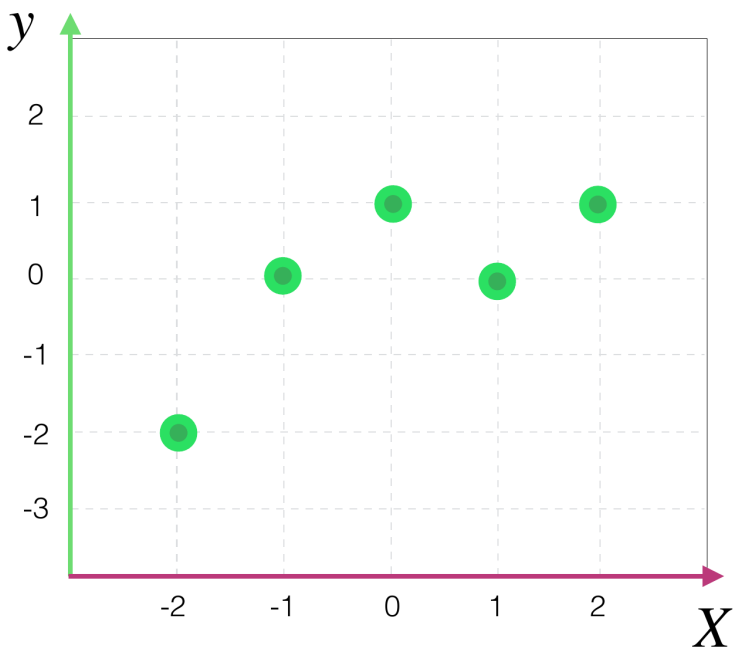
S

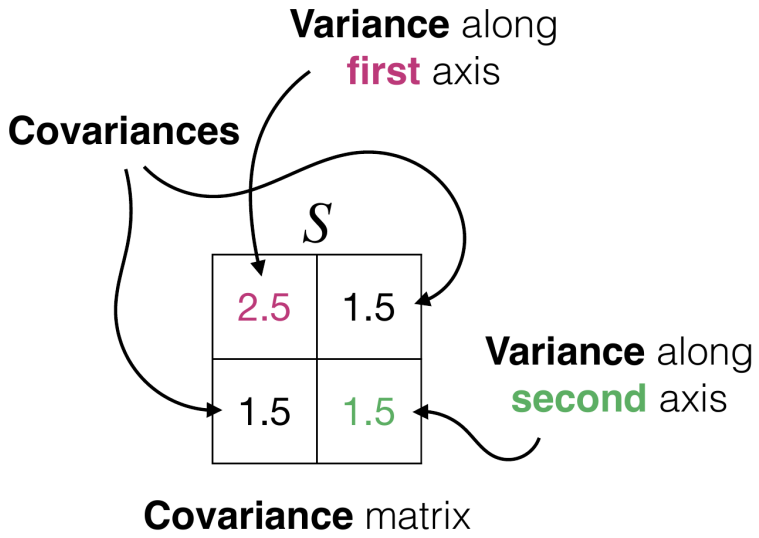
2.5	1.5
1.5	1.5

Covariance matrix

Principal Component Analysis

How to **interpret** values in **covariance** matrix?





Principal Component Analysis

Z^T

-2	-1	0	1	2
-2	0	1	0	1

$\times$

Z

-2	-2
-1	0
0	1
1	0
2	1

$=$

S

2.5	1.5
1.5	1.5

$\times 4$

Principal Component Analysis

$$S = \begin{bmatrix} 2.5 & 1.5 \\ 1.5 & 1.5 \end{bmatrix} = PDP^{\top}$$

Principal Component Analysis

$$S = PDP^{\top}$$

$$\begin{bmatrix} 2.5 & 1.5 \\ 1.5 & 1.5 \end{bmatrix} = \begin{bmatrix} 2.5 & 1.5 \\ 1.5 & 1.5 \end{bmatrix}$$

For an example: https://www.scss.tcd.ie/Rozenn.Dahyot/CS1BA1/SolutionEigen.pdf

Principal Component Analysis

$$
\underset{S}{\begin{bmatrix} 2.5 & 1.5 \\ 1.5 & 1.5 \end{bmatrix}} = \underset{PD}{\begin{bmatrix} -2.9 & 0.24 \\ -2.1 & -0.33 \end{bmatrix}} \times \underset{P^{\top}}{\begin{bmatrix} -0.81 & -0.58 \\ 0.58 & -0.81 \end{bmatrix}}
$$

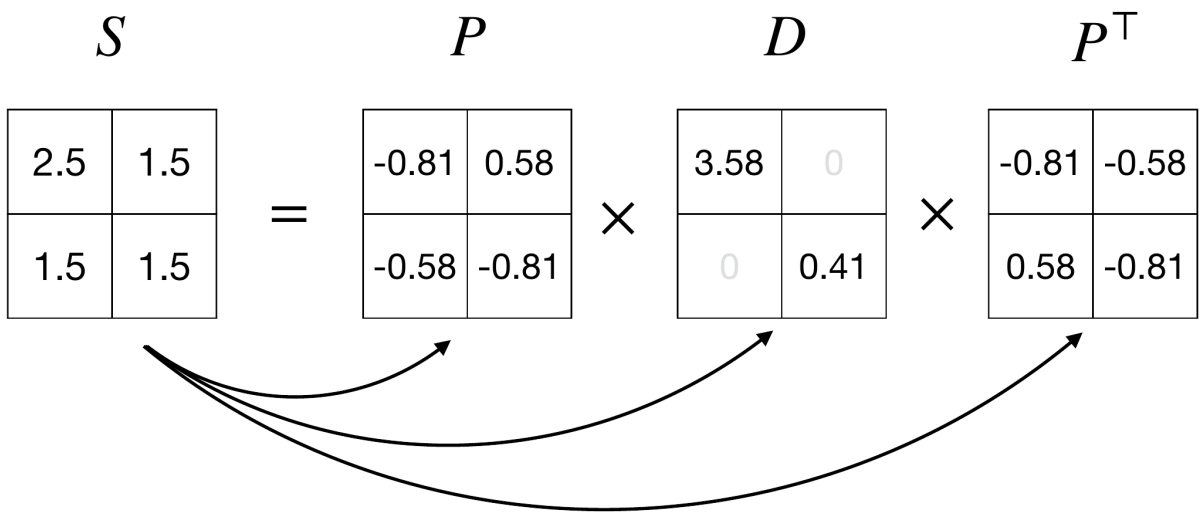
For an example: https://www.scss.tcd.ie/Rozenn.Dahyot/CS1BA1/SolutionEigen.pdf

Principal Component Analysis

$$
\underset{S}{\begin{bmatrix} 2.5 & 1.5 \\ 1.5 & 1.5 \end{bmatrix}} = \underset{P}{\begin{bmatrix} -0.81 & 0.58 \\ -0.58 & -0.81 \end{bmatrix}} \times \underset{D}{\begin{bmatrix} 3.58 & 0 \\ 0 & 0.41 \end{bmatrix}} \times \underset{P^{\top}}{\begin{bmatrix} -0.81 & -0.58 \\ 0.58 & -0.81 \end{bmatrix}}
$$

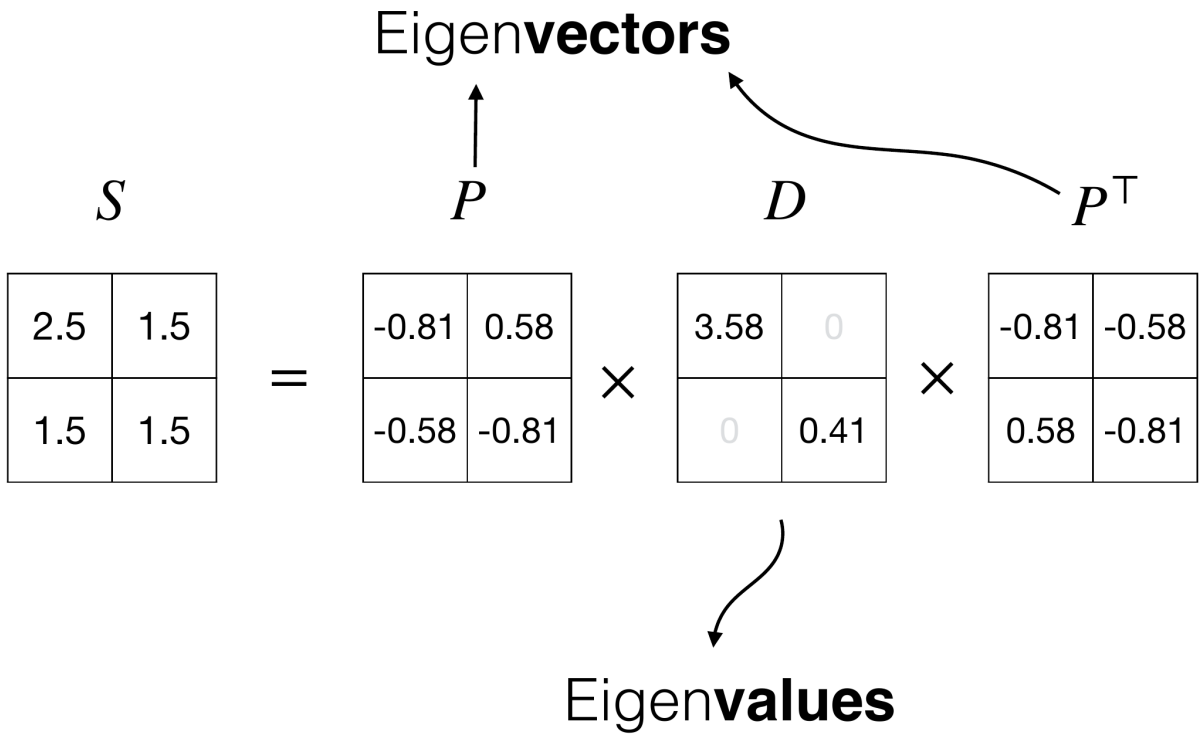
For an example: https://www.scss.tcd.ie/Rozenn.Dahyot/CS1BA1/SolutionEigen.pdf

Eigen**decomposition**



For an example: https://www.scss.tcd.ie/Rozenn.Dahyot/CS1BA1/SolutionEigen.pdf

Eigen**decomposition**

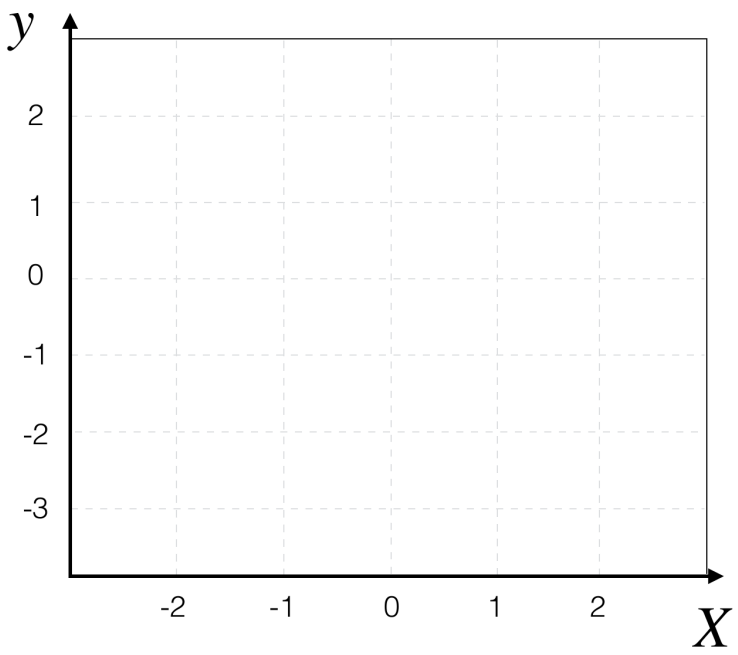


For an example: https://www.scss.tcd.ie/Rozenn.Dahyot/CS1BA1/SolutionEigen.pdf

Principal Component Analysis

Eigen**vectors**

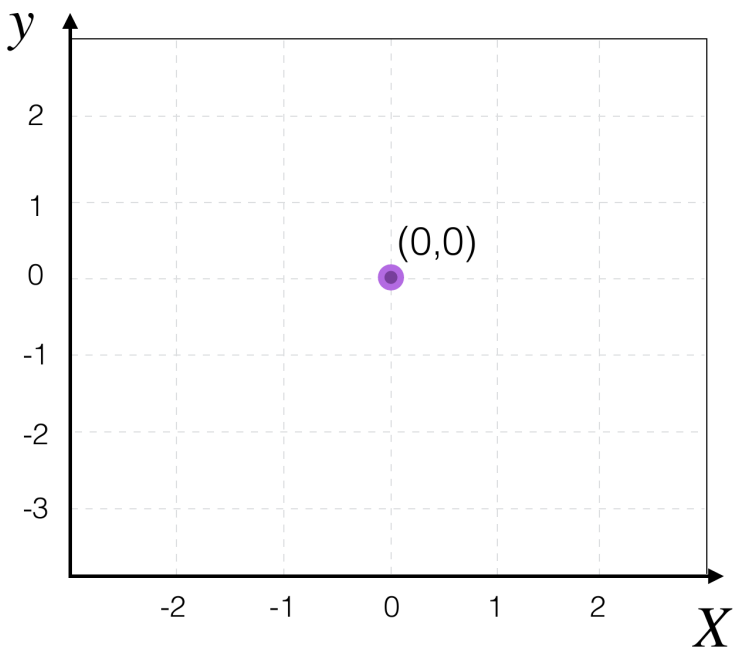
-0.81	0.58
-0.58	-0.81



Principal Component Analysis

Eigen**vectors**

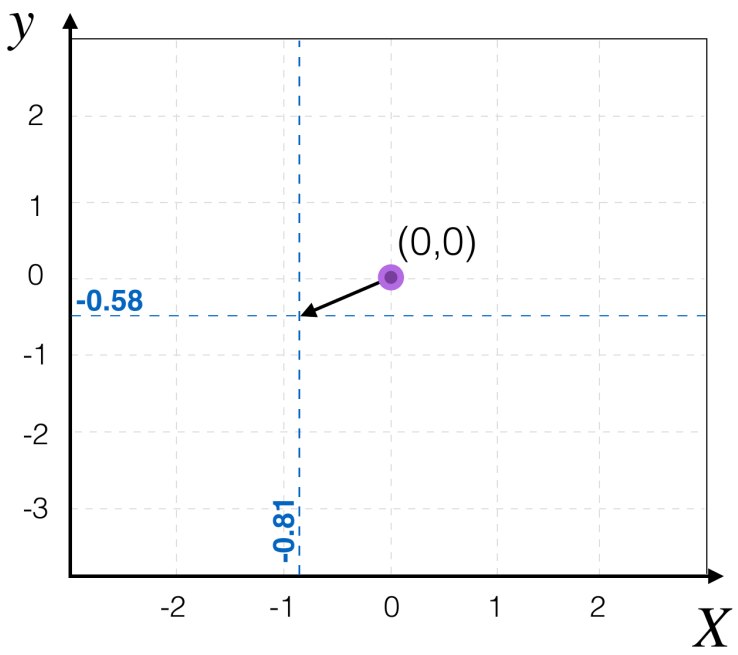
-0.81	0.58
-0.58	-0.81



Principal Component Analysis

Eigen**vectors**

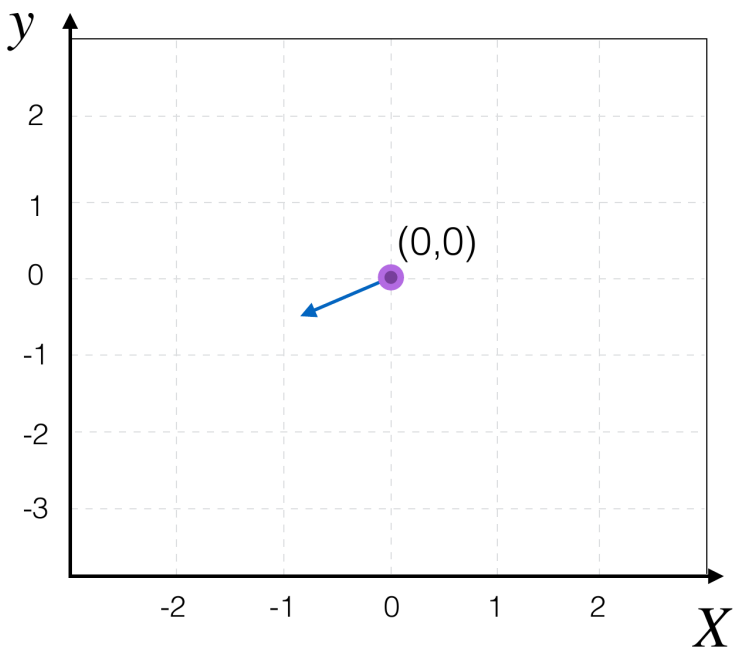
-0.81	0.58
-0.58	-0.81



Principal Component Analysis

Eigen**vectors**

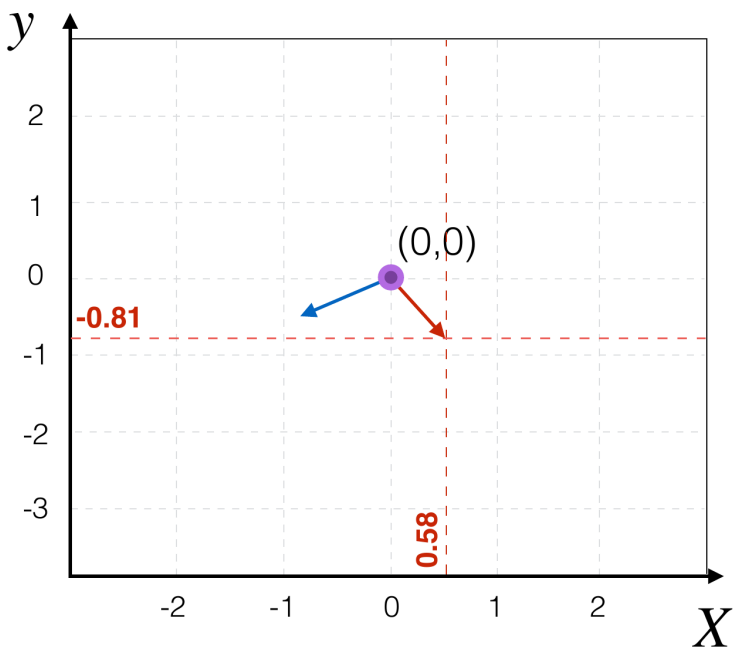
-0.81	0.58
-0.58	-0.81



Principal Component Analysis

Eigen**vectors**

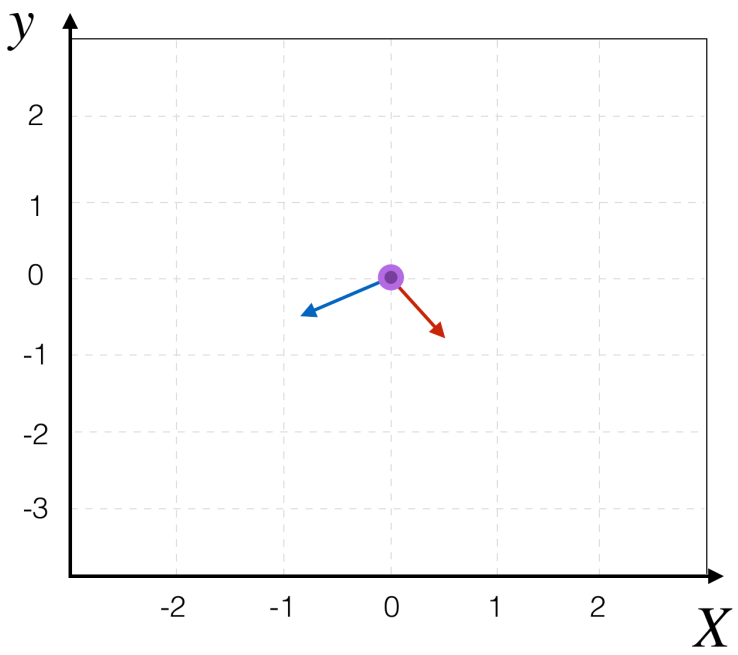
-0.81	0.58
-0.58	-0.81



Principal Component Analysis

Eigen**vectors**

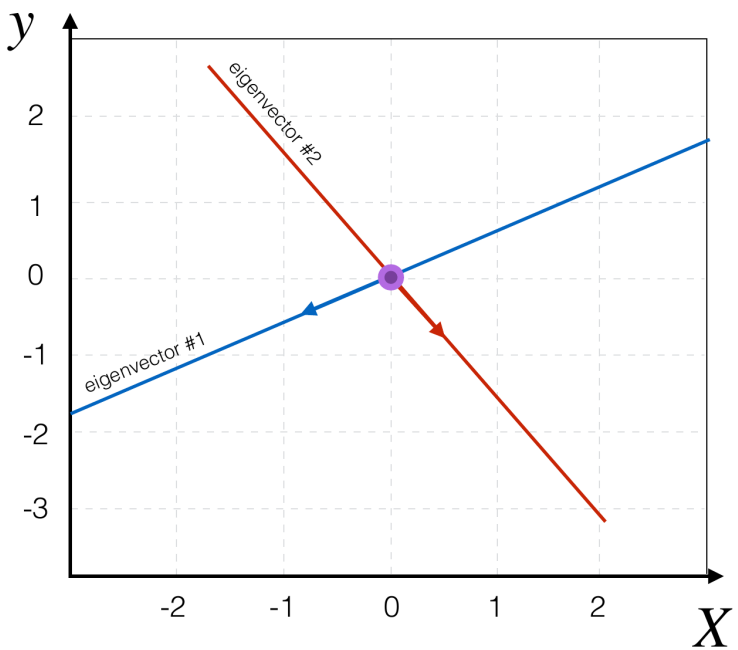
-0.81	0.58
-0.58	-0.81



Principal Component Analysis

Eigen**vectors**

-0.81	0.58
-0.58	-0.81

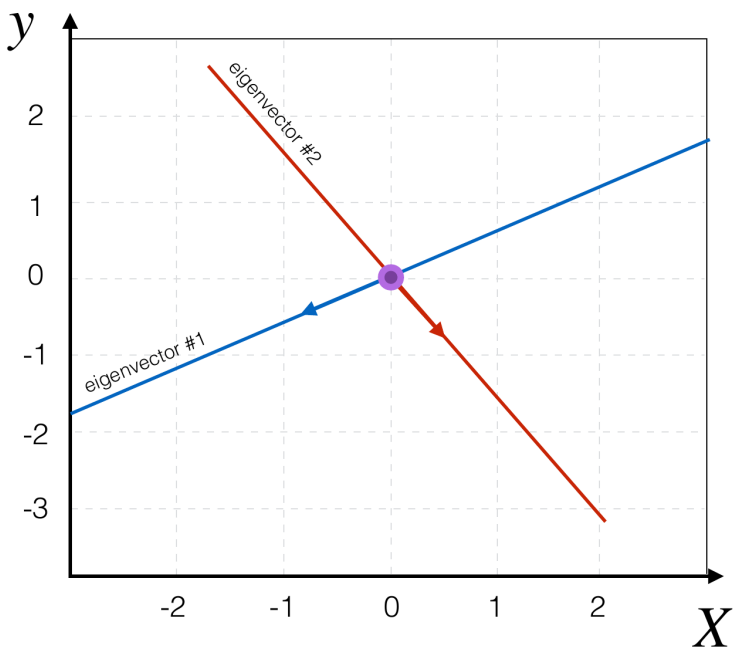


Old coordinate system

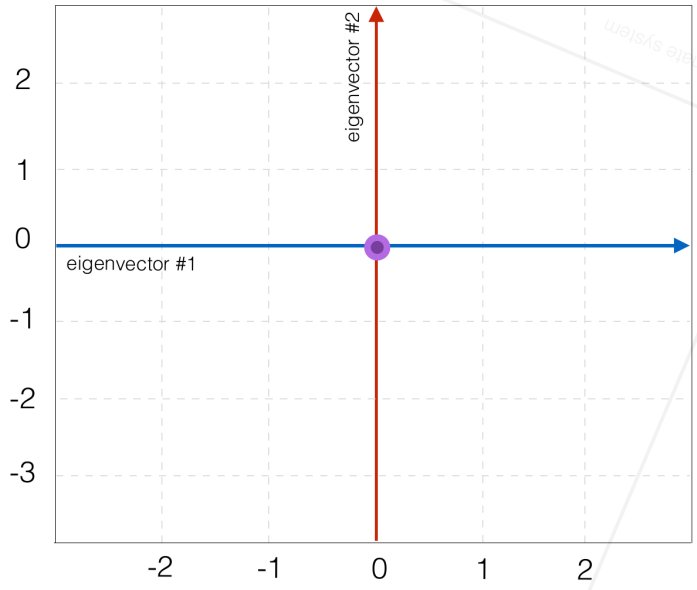
Principal Component Analysis

Eigen**vectors**

-0.81	0.58
-0.58	-0.81



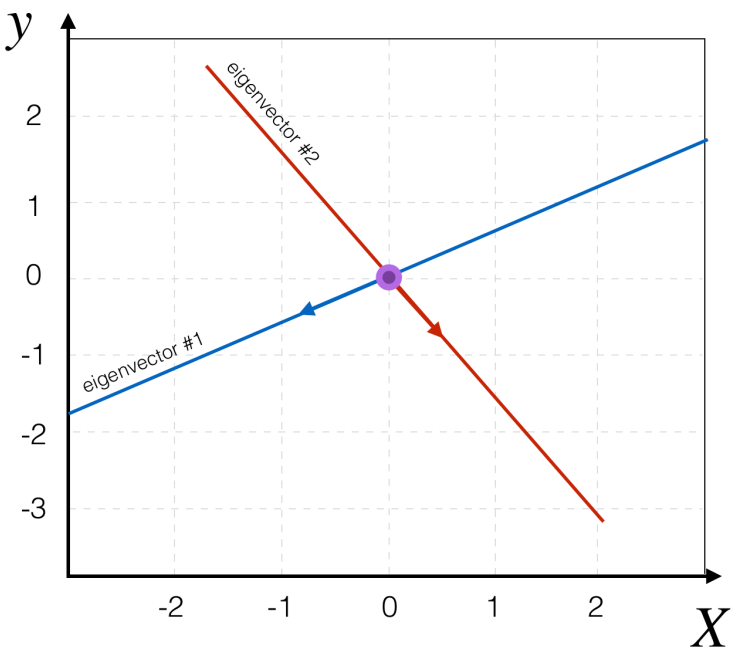
Old coordinate system



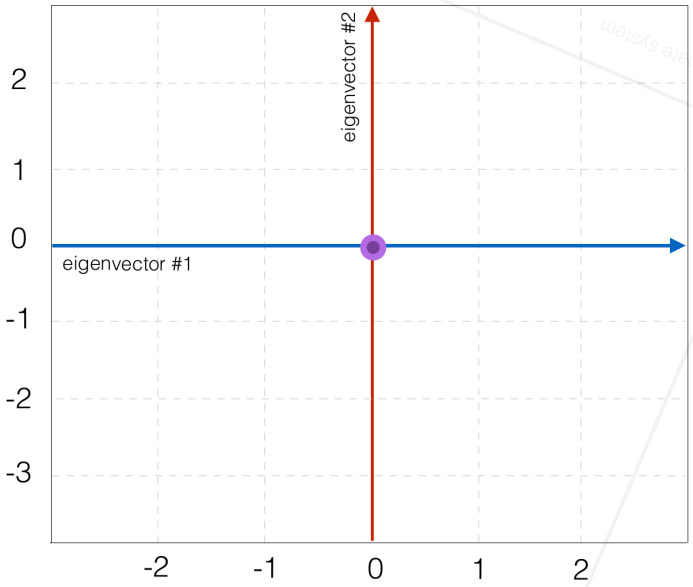
New coordinate system

Principal Component Analysis

Eigen**vectors**		transpose	Eigen**vectors**^{T}	
-0.81	0.58	=	-0.81	-0.58
-0.58	-0.81		0.58	-0.81



Old coordinate system

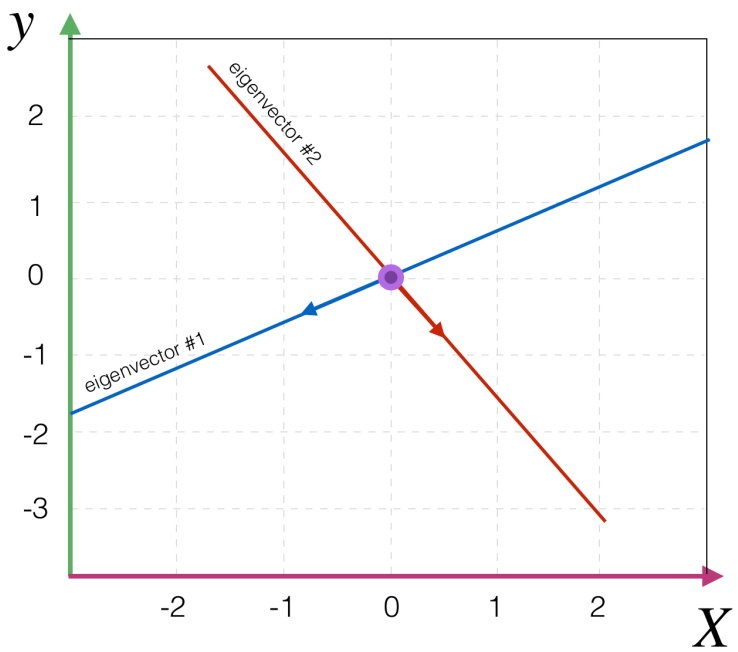


New coordinate system

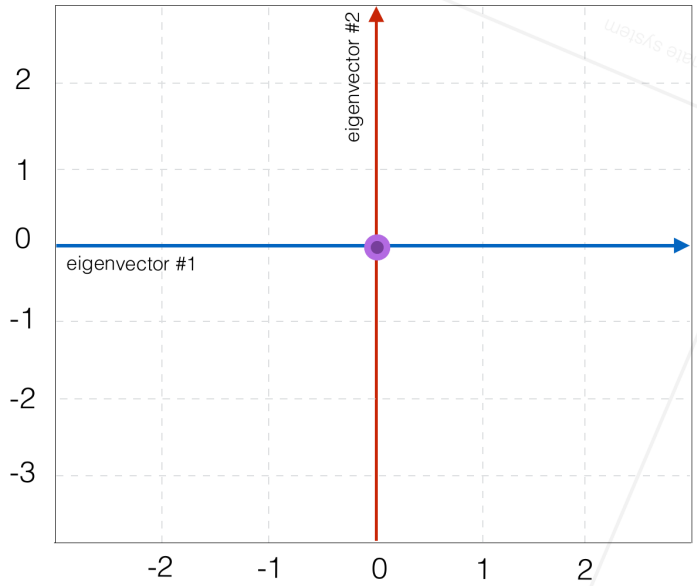
Principal Component Analysis

Eigen**vectors**$^{\mathsf{T}}$

-0.81	-0.58
0.58	-0.81



Old coordinate system



New coordinate system

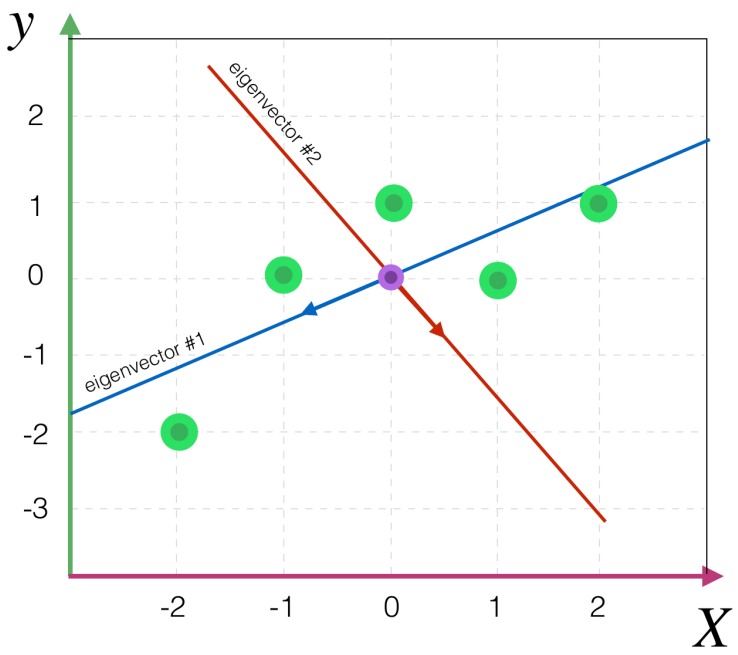
Principal Component Analysis

Eigen**vectors**$^{\mathsf{T}}$

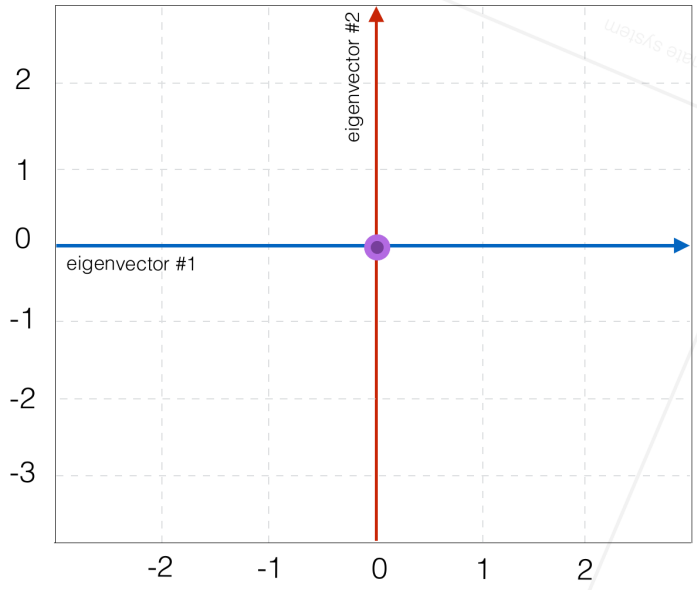
-0.81	-0.58
0.58	-0.81

Z^{T}

-2	-1	0	1	2
-2	0	1	0	1



Old coordinate system



New coordinate system

Principal Component Analysis

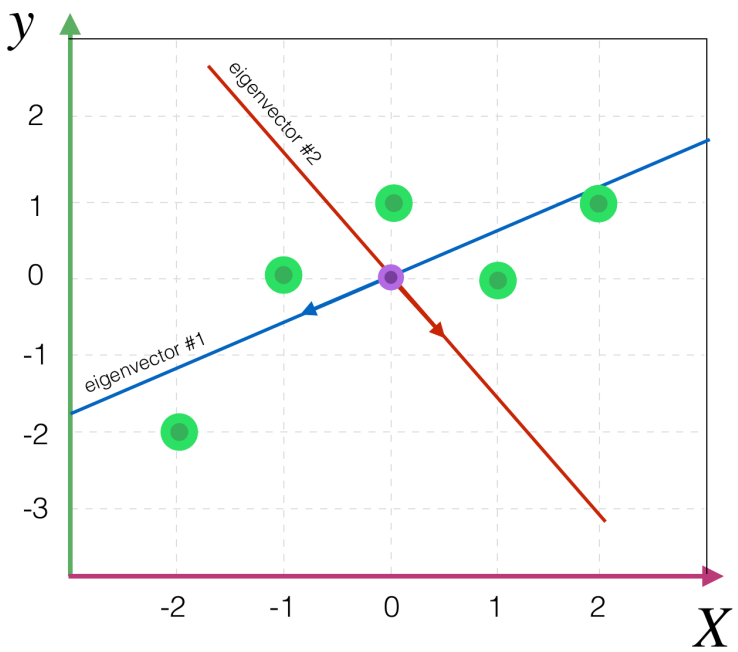
Eigen**vectors**$^{\mathsf{T}}$

-0.81	-0.58
0.58	-0.81

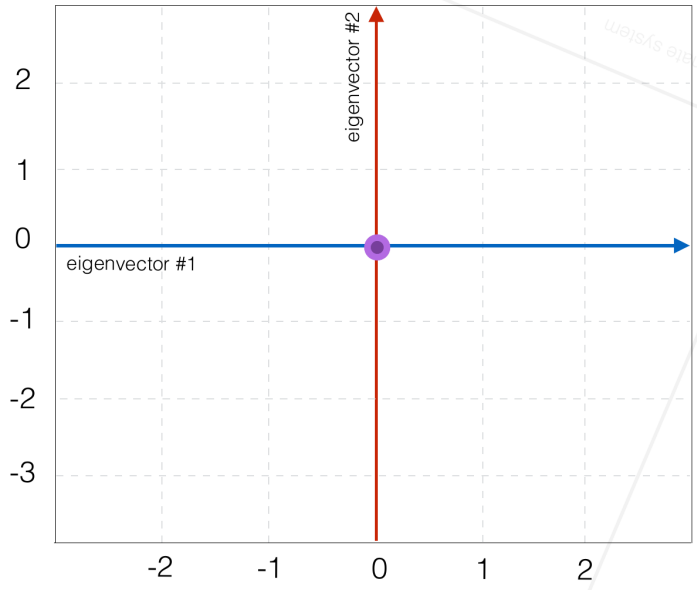
$\times$

Z^{T}

-2	-1	0	1	2
-2	0	1	0	1



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\mathsf{T}}$

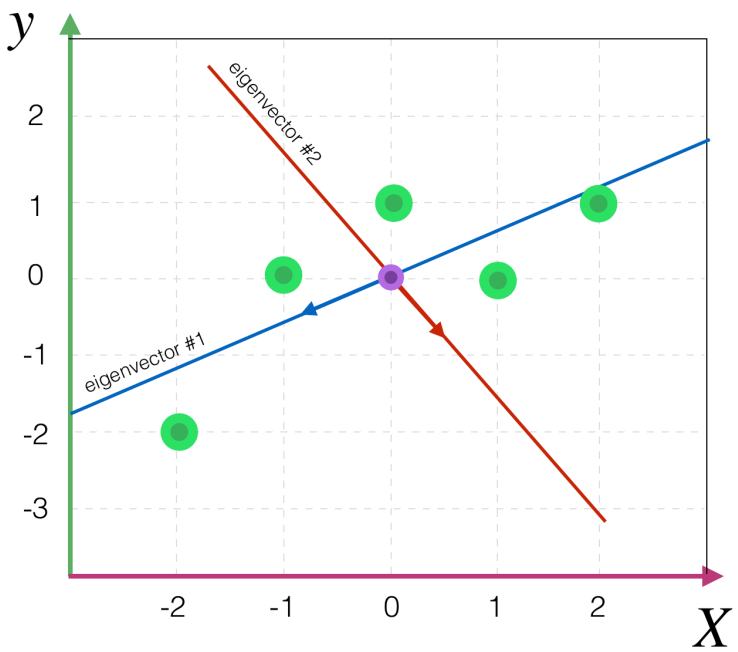
-0.81	-0.58
0.58	-0.81

$\times$

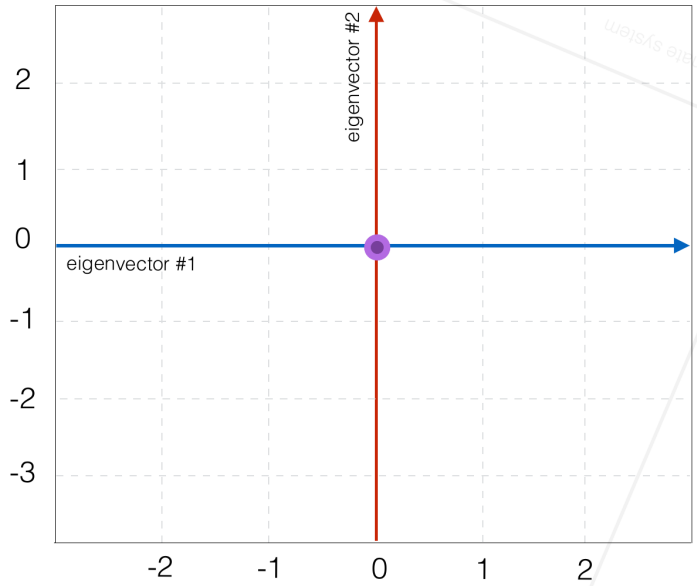
Z^{T}

-2	-1	0	1	2
-2	0	1	0	1

$=$



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\top}$

-0.81	-0.58
0.58	-0.81

$\times$

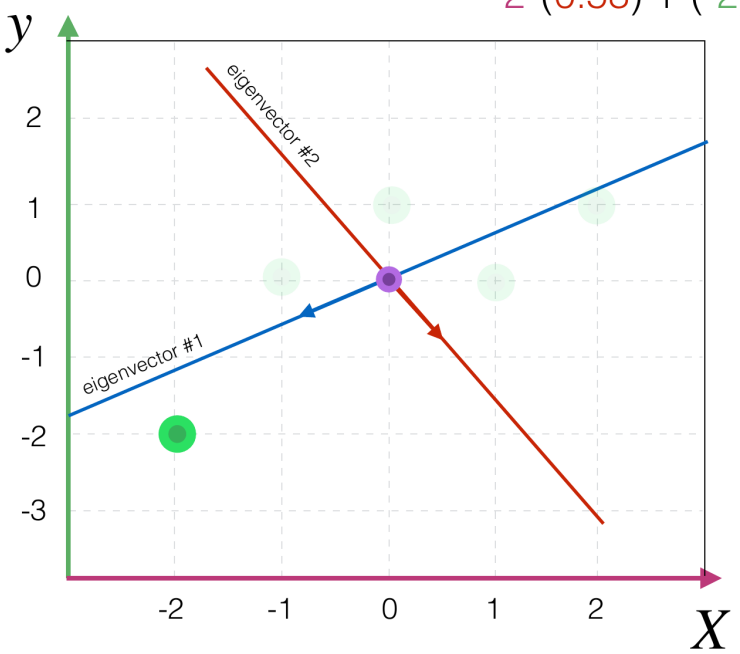
$Z^{\top}$

-2	-1	0	1	2
-2	0	1	0	1

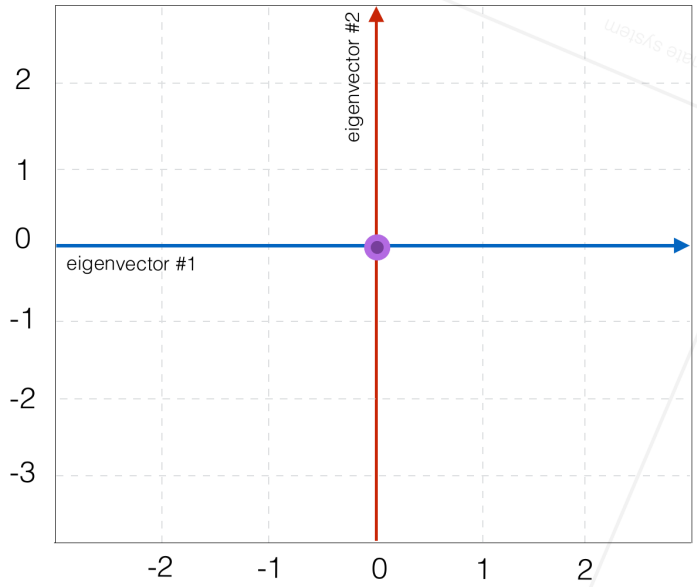
$=$

-2*(-0.81) + (-2)*(-0.58) = **2.78**

-2*(0.58) + (-2)*(-0.81) = **0.46**



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\top}$

-0.81	-0.58
0.58	-0.81

$\times$

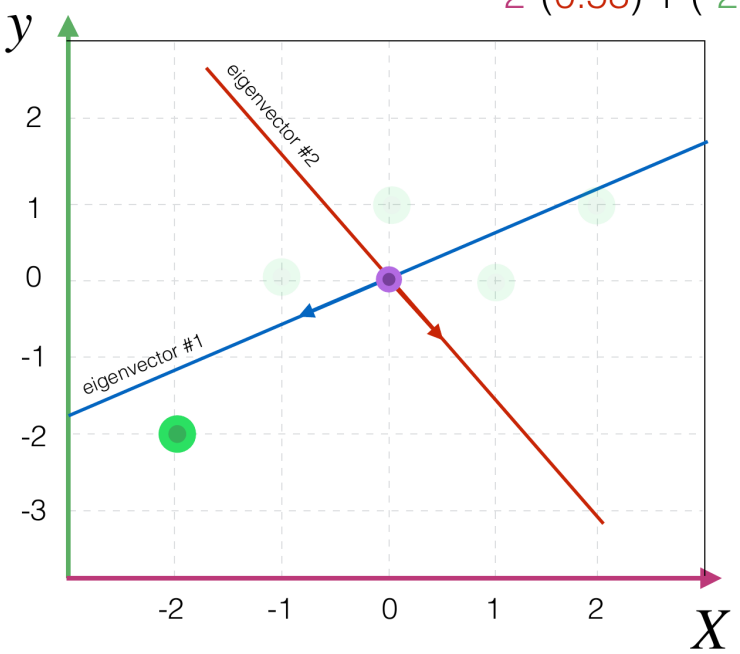
$Z^{\top}$

-2	-1	0	1	2
-2	0	1	0	1

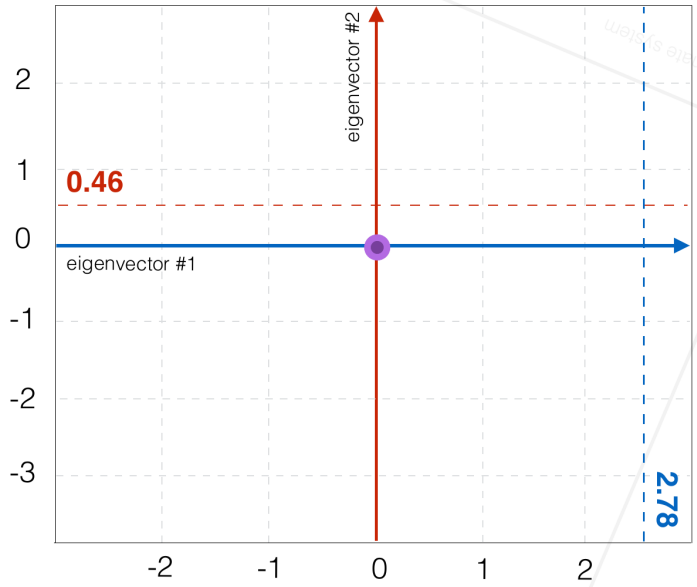
$=$

-2*(-0.81) + (-2)*(-0.58) = **2.78**

-2*(0.58) + (-2)*(-0.81) = **0.46**

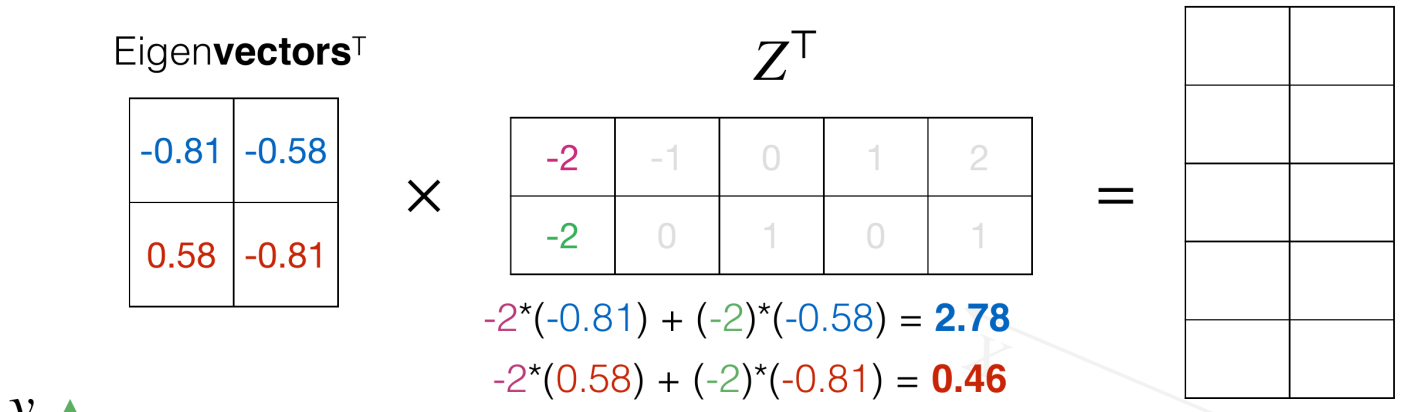


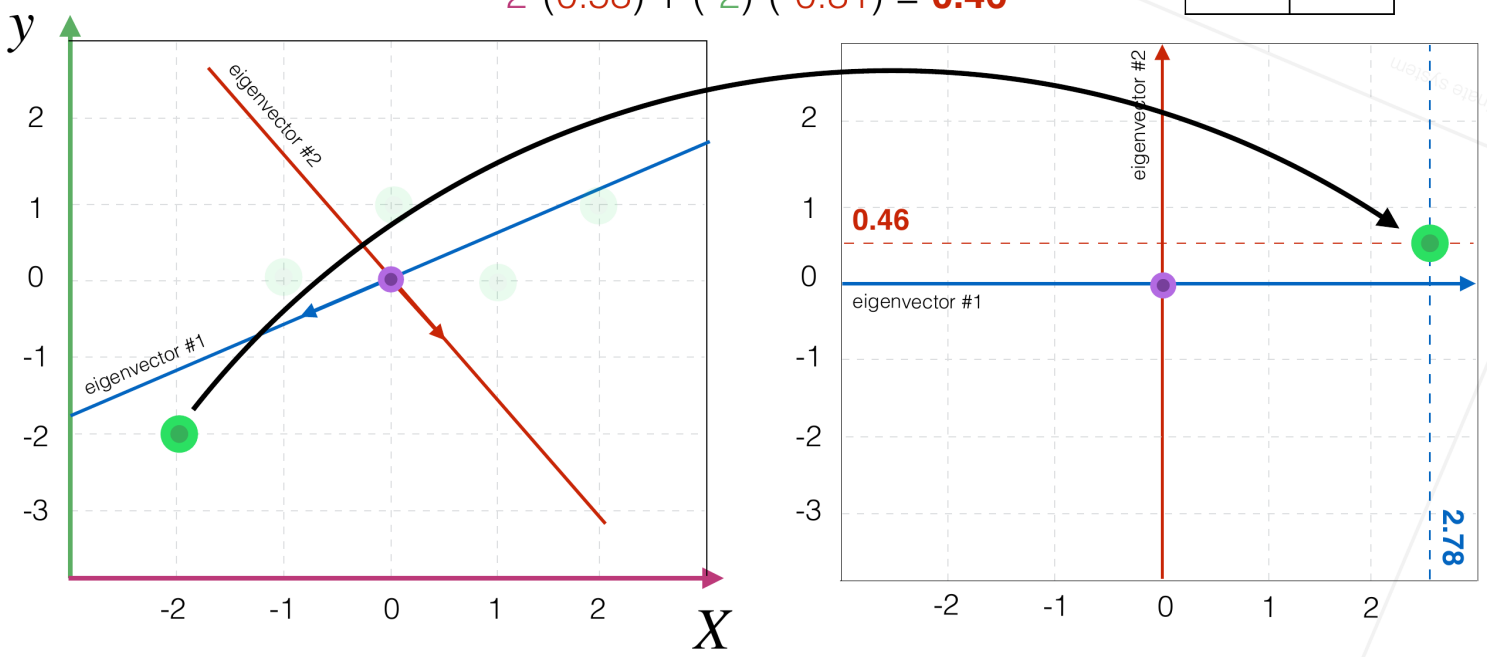
Old coordinate system



New coordinate system

Principal Component Analysis





Old coordinate system

New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\mathsf{T}}$

-0.81	-0.58
0.58	-0.81

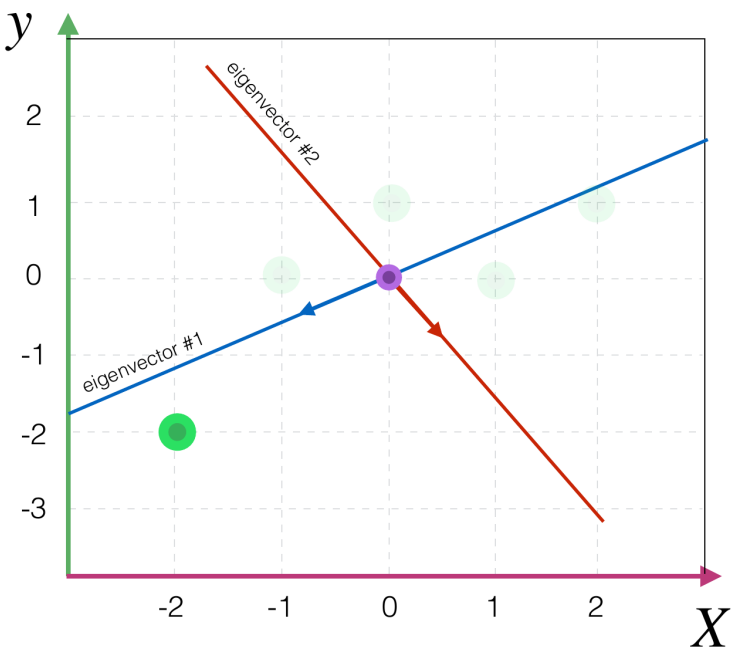
$\times$

Z^{T}

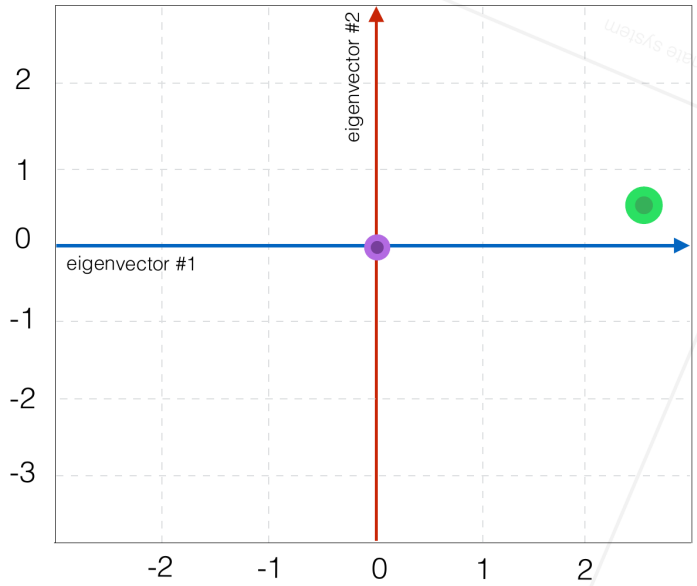
-2	-1	0	1	2
-2	0	1	0	1

$=$

2.78	0.46



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\top}$

-0.81	-0.58
0.58	-0.81

$\times$

$Z^{\top}$

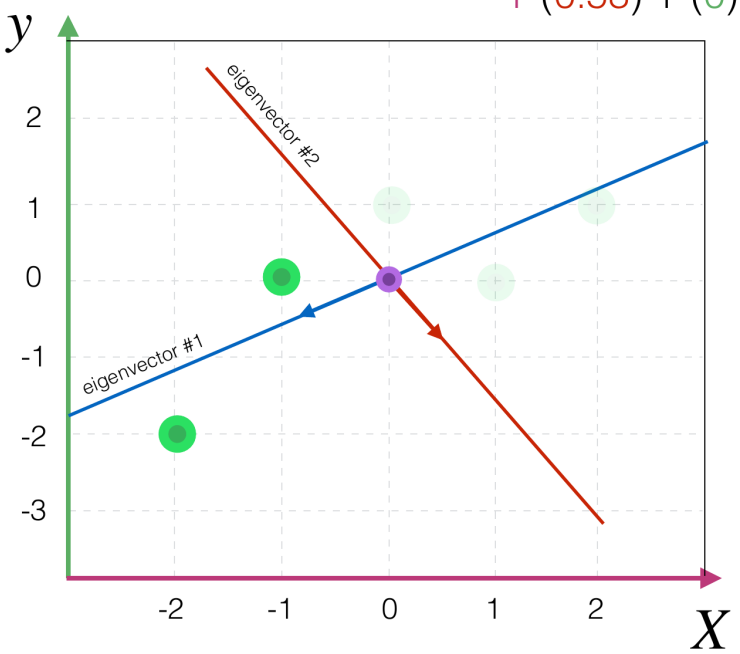
-2	-1	0	1	2
-2	0	1	0	1

$=$

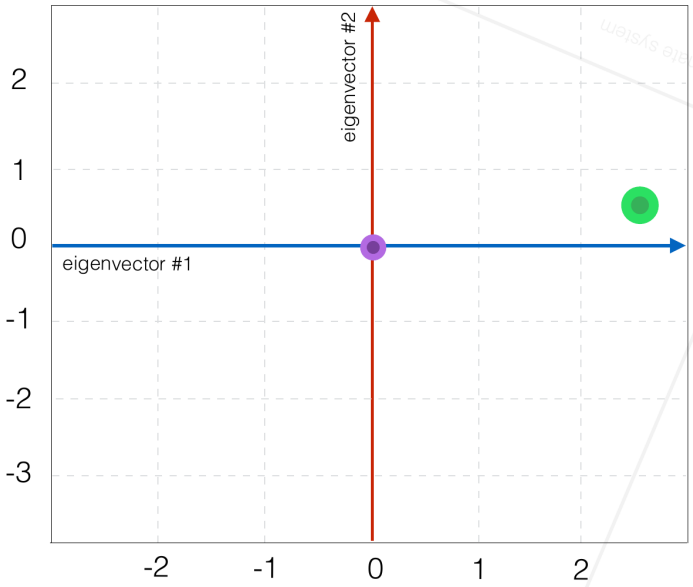
2.78	0.46

-1*(-0.81) + (0)*(-0.58) = **0.81**

-1*(0.58) + (0)*(-0.81) = **-0.58**



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\top}$

-0.81	-0.58
0.58	-0.81

$\times$

$Z^{\top}$

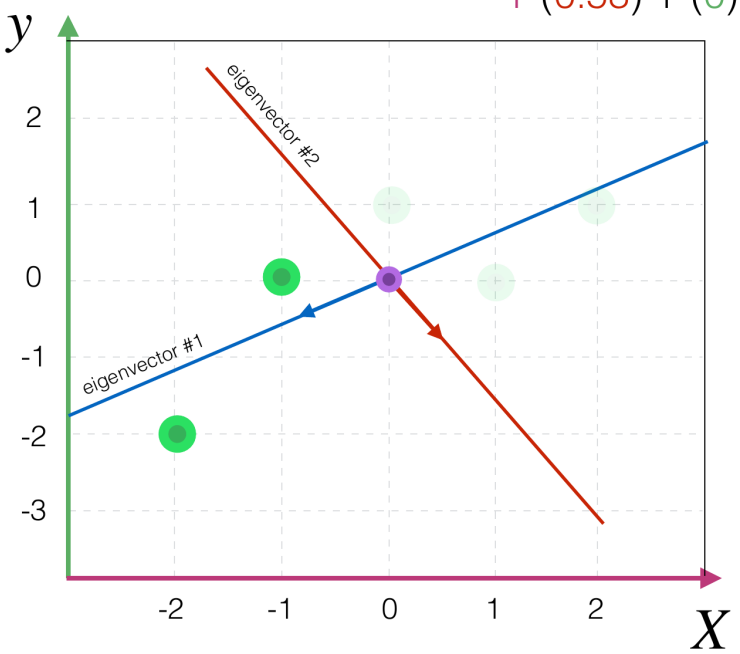
-2	-1	0	1	2
-2	0	1	0	1

$=$

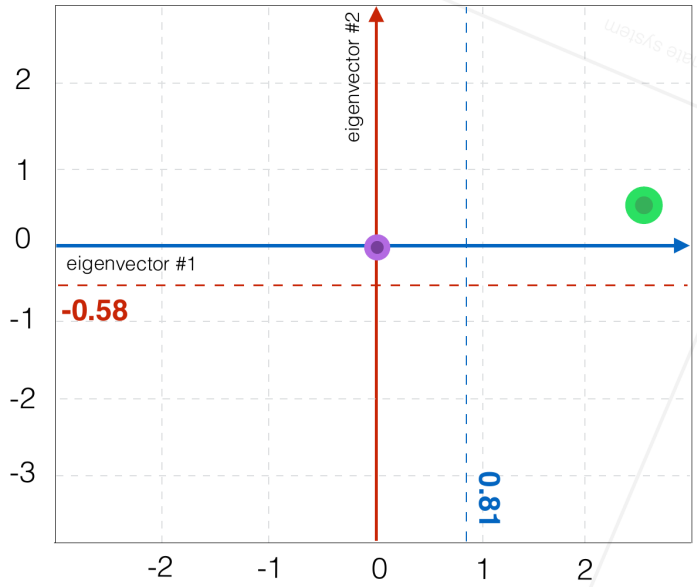
2.78	0.46

-1*(-0.81) + (0)*(-0.58) = **0.81**

-1*(0.58) + (0)*(-0.81) = **-0.58**



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\top}$

-0.81	-0.58
0.58	-0.81

$\times$

$Z^{\top}$

-2	-1	0	1	2
-2	0	1	0	1

$=$

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0.81	-0.58

-1*(-0.81) + (0)*(-0.58) = **0.81**

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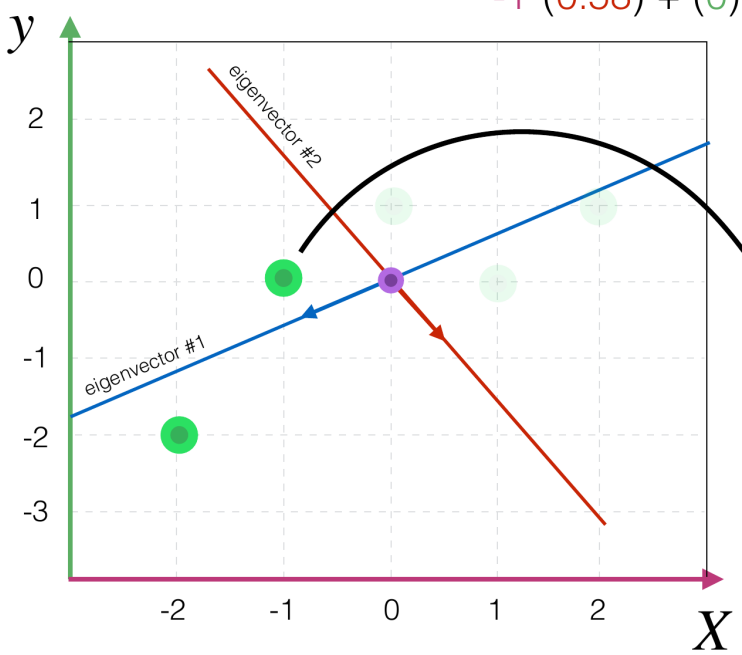
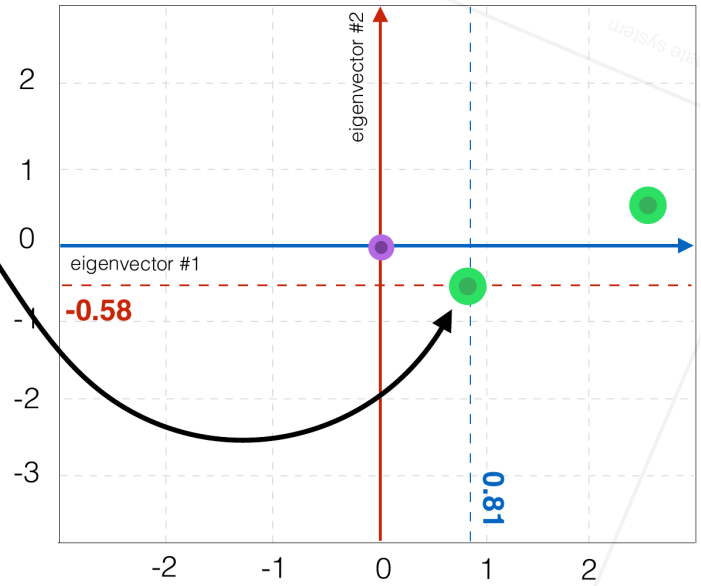


Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\mathsf{T}}$

-0.81	-0.58
0.58	-0.81

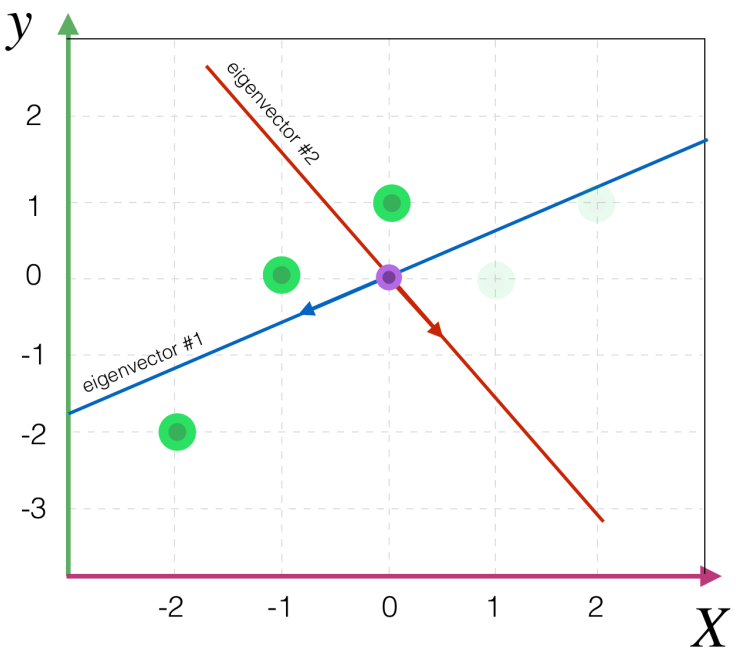
$\times$

Z^{T}

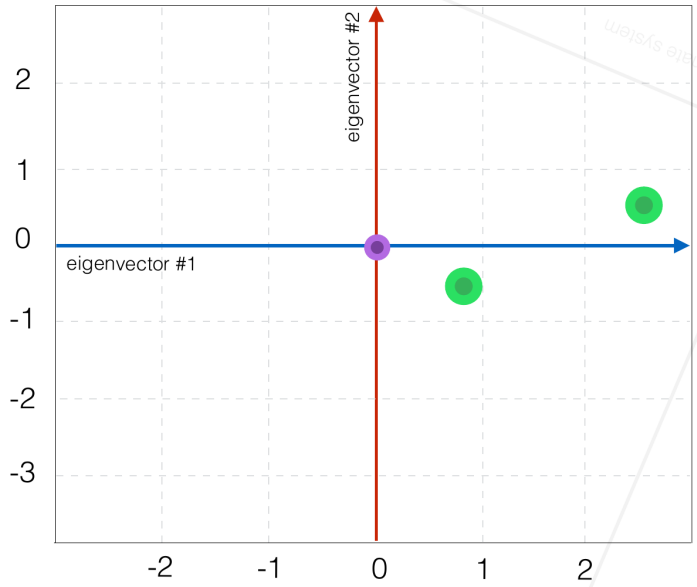
-2	-1	0	1	2
-2	0	1	0	1

$=$

2.78	0.46
0.81	-0.58



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\top}$

-0.81	-0.58
0.58	-0.81

$\times$

$Z^{\top}$

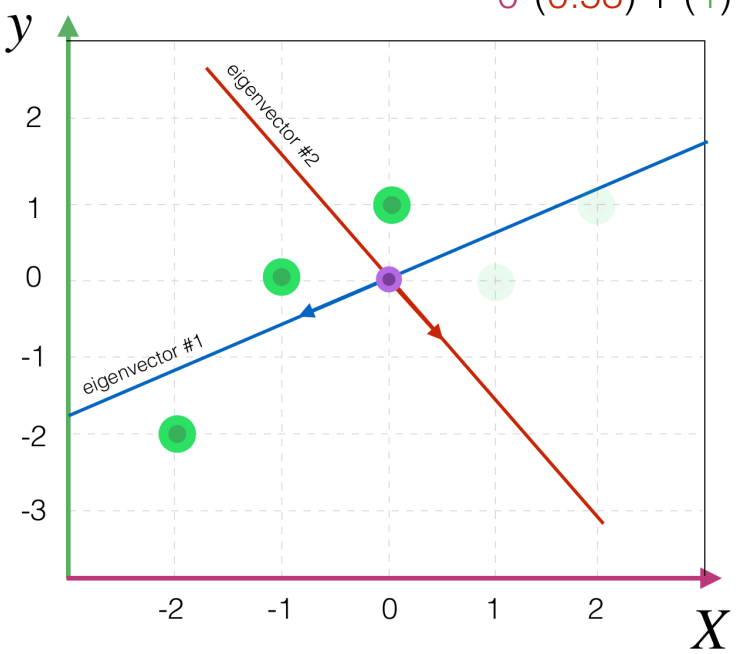
-2	-1	0	1	2
-2	0	1	0	1

$=$

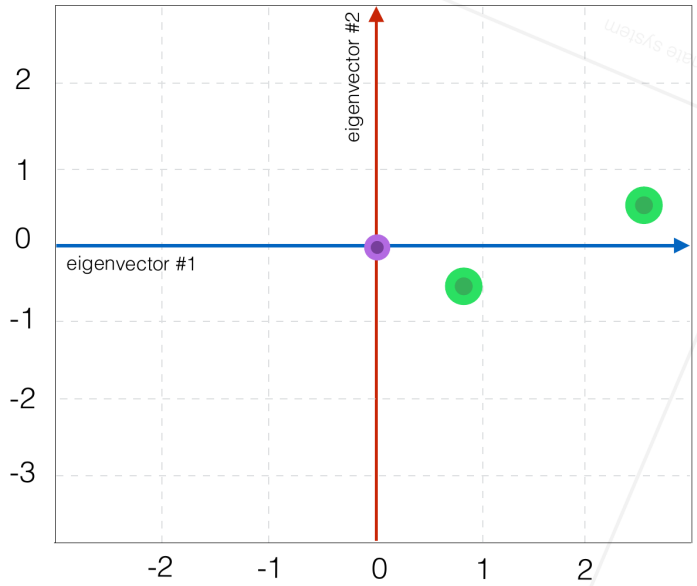
2.78	0.46
0.81	-0.58

0*(-0.81) + (1)*(-0.58) = **-0.58**

0*(0.58) + (1)*(-0.81) = **-0.81**



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\top}$

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0.58	-0.81

$\times$

$Z^{\top}$

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$=$

2.78	0.46
0.81	-0.58
-0.58	-0.81

0*(-0.81) + (1)*(-0.58) = **-0.58**

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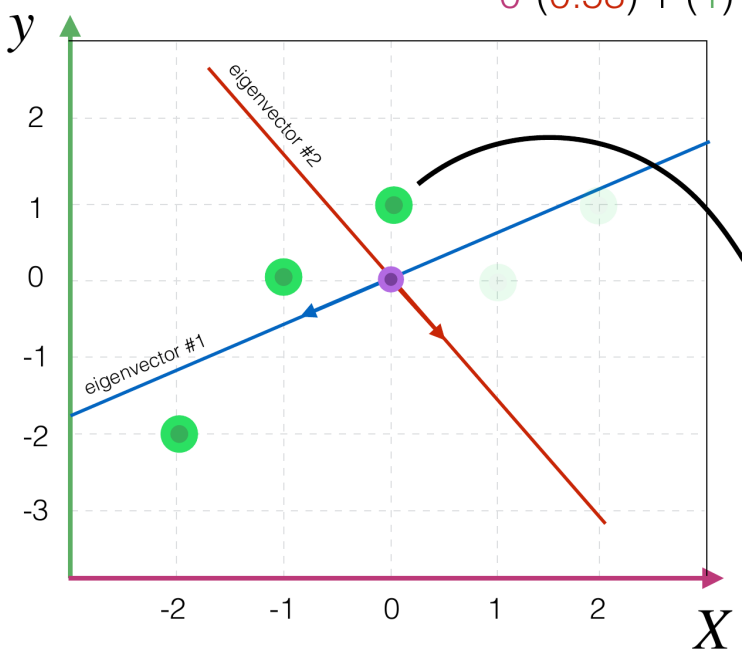
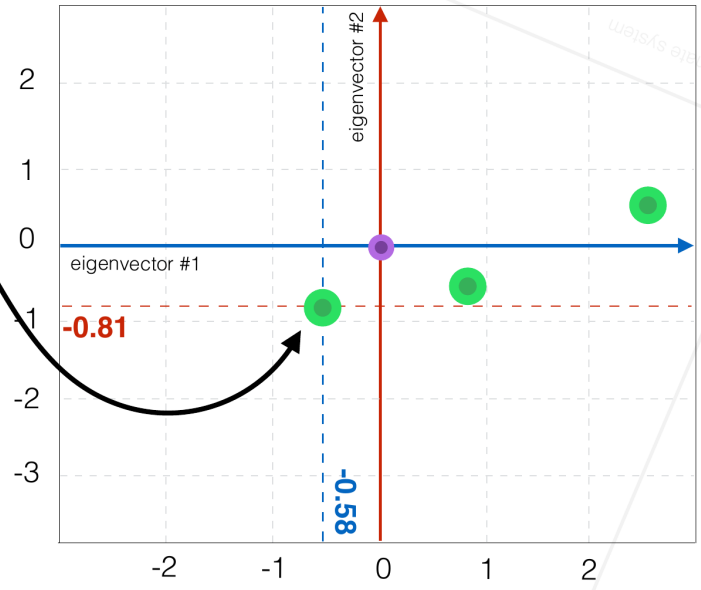


Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\mathsf{T}}$

-0.81	-0.58
0.58	-0.81

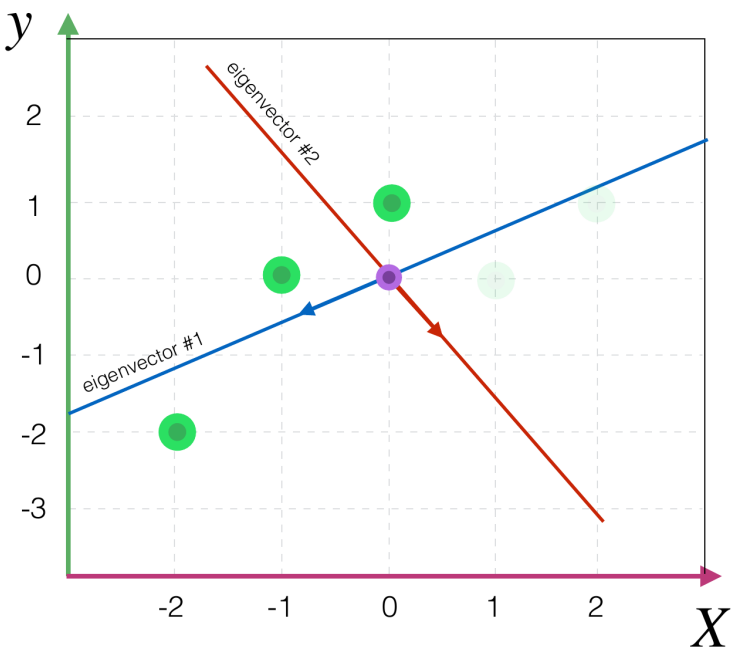
$\times$

Z^{T}

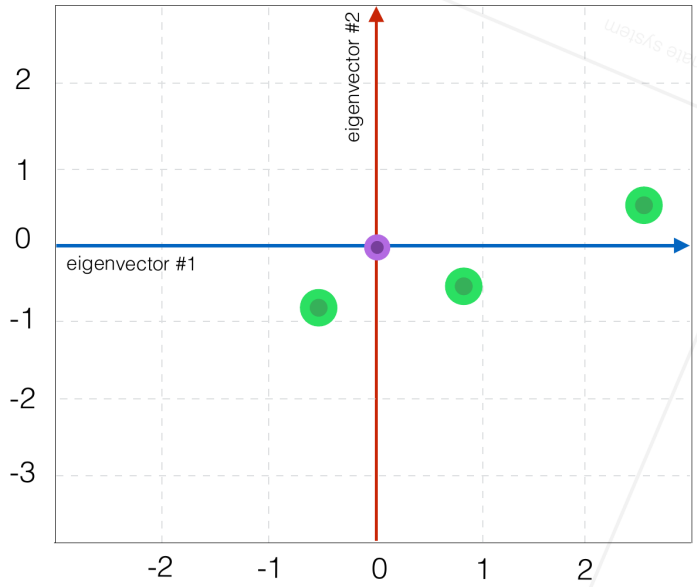
-2	-1	0	1	2
-2	0	1	0	1

$=$

2.78	0.46
0.81	-0.58
-0.58	-0.81



Old coordinate system



New coordinate system

Principal Component Analysis

Eigen**vectors**$^{\mathsf{T}}$

-0.81	-0.58
0.58	-0.81

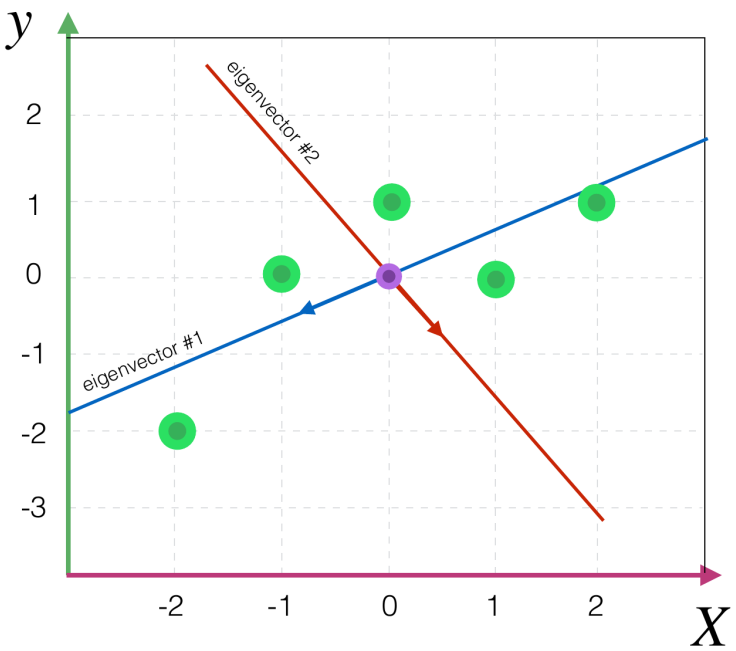
$\times$

Z^{T}

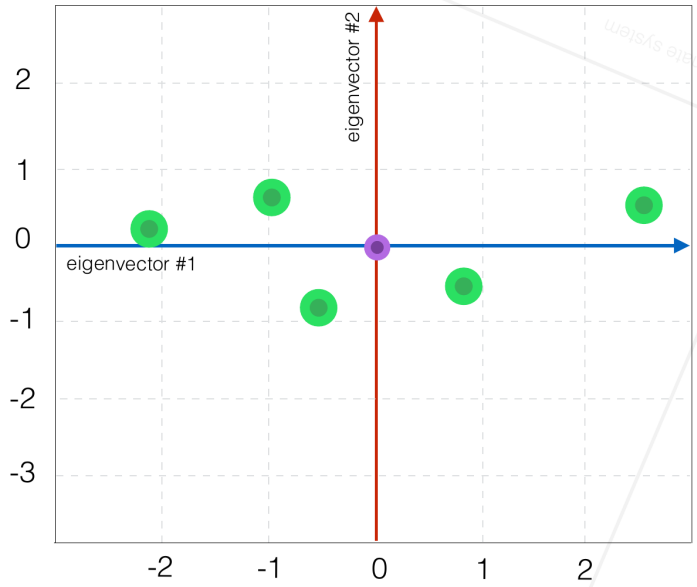
-2	-1	0	1	2
-2	0	1	0	1

$=$

2.78	0.46
0.81	-0.58
-0.58	-0.81
-0.81	0.58
-2.2	0.35



Old coordinate system



New coordinate system

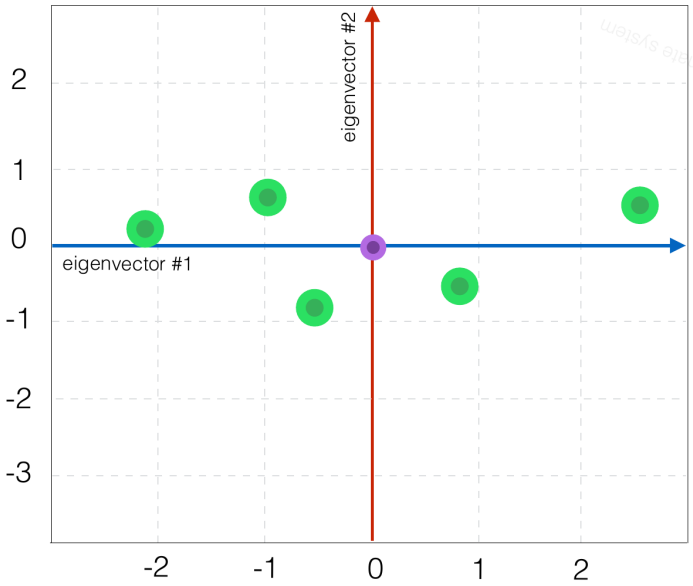
Principal Component Analysis

These eigenvectors are called **P**rinciple **C**omponents

2.78	0.46
0.81	-0.58
-0.58	-0.81
-0.81	0.58
-2.2	0.35

eigenvector #1 is called **PC1**

eigenvector #2 is called **PC2**



New coordinate system

Principal Component Analysis

These eigenvectors are called **P**rinciple **C**omponents

2.78	0.46
0.81	-0.58
-0.58	-0.81
-0.81	0.58
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eigenvector #1 is called **PC1**

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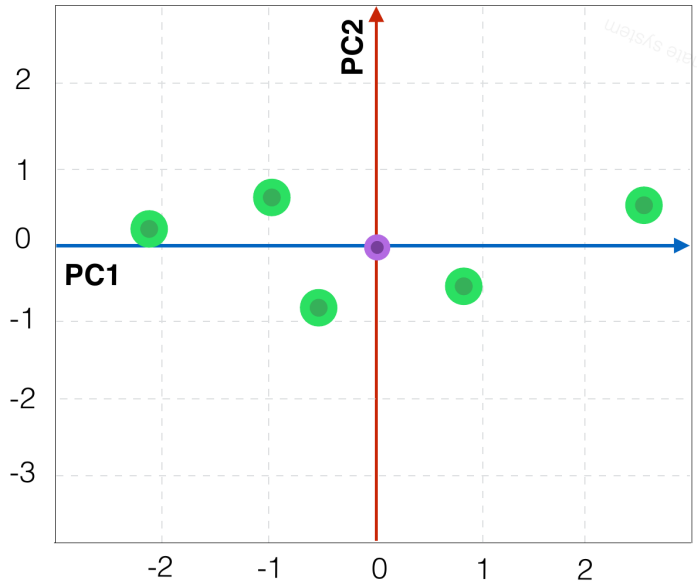
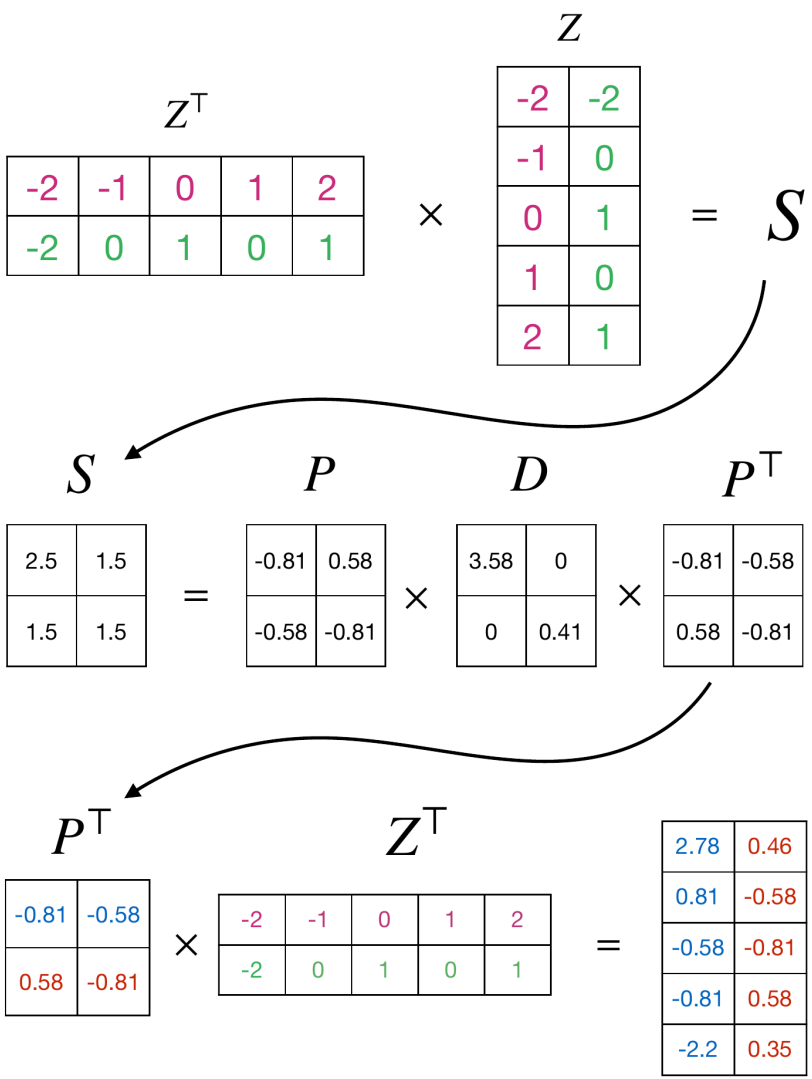


New coordinate system

Principal Component Analysis



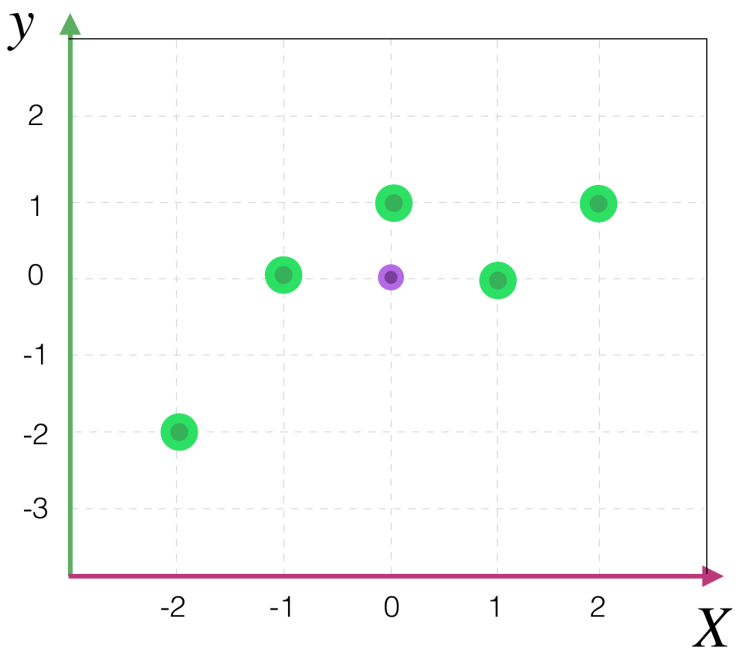
Compute **covariance** matrix

Perform **eigen**decomposition

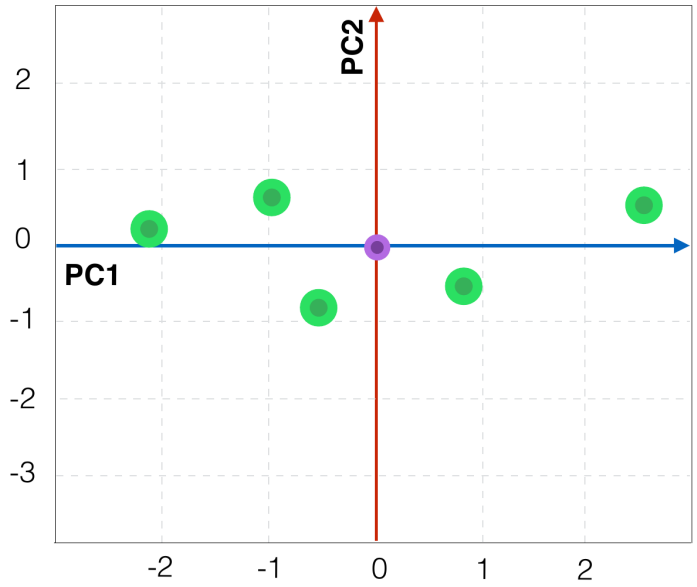
Compute new **coordinates**

Principal Component Analysis

Do you still remember what was it all about?



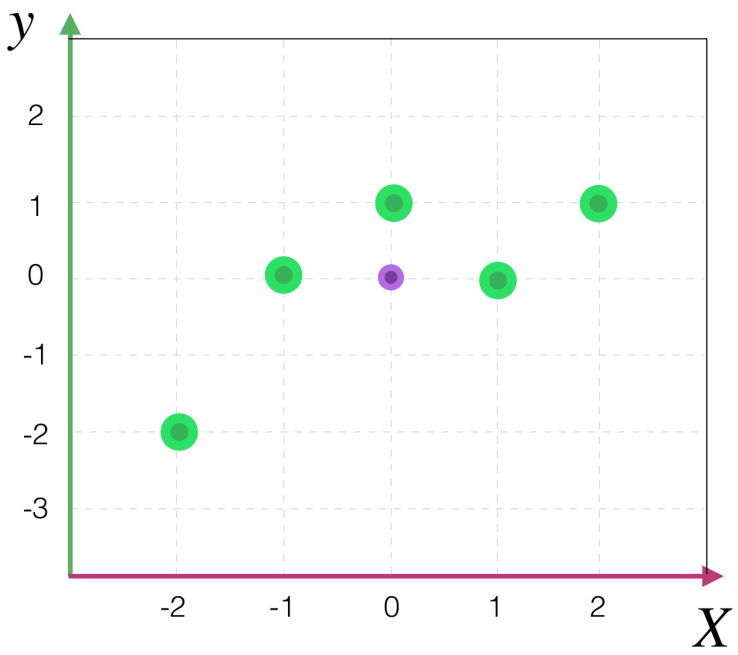
Old coordinate system



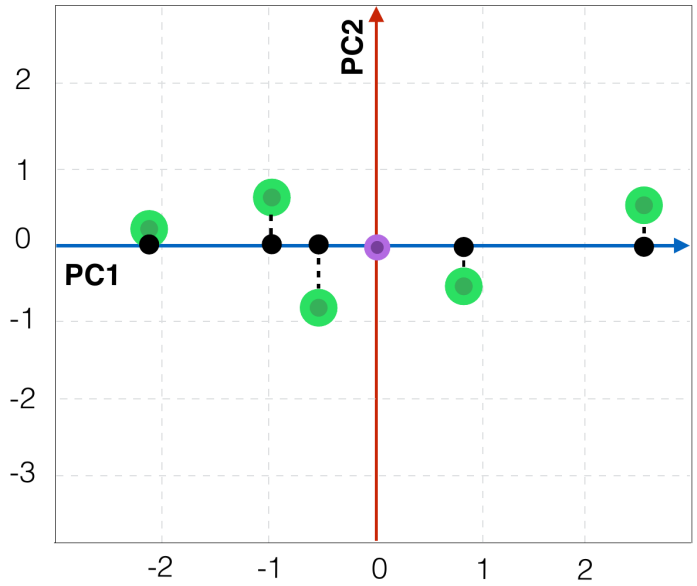
New coordinate system

Principal Component Analysis

Do you still remember what was it all about?
We want to **reduce the dimensionality**!



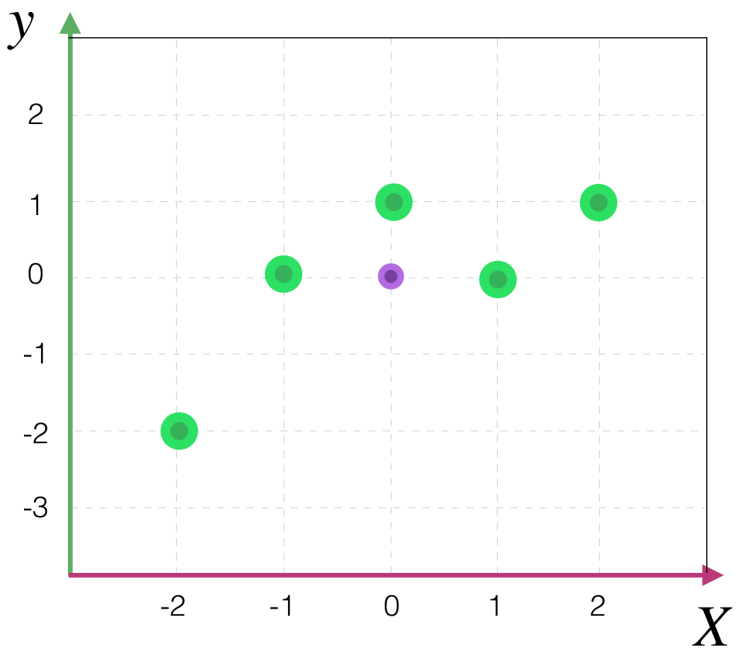
Old coordinate system



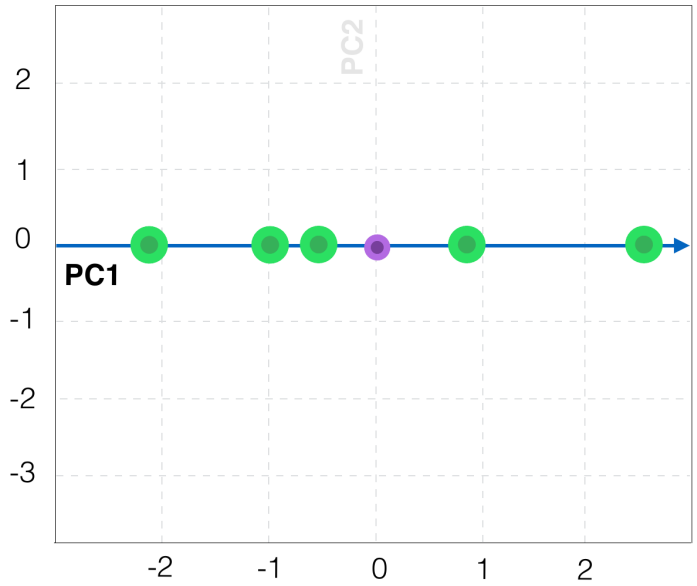
New coordinate system

Principal Component Analysis

Do you still remember what was it all about?
We want to **reduce the dimensionality**!



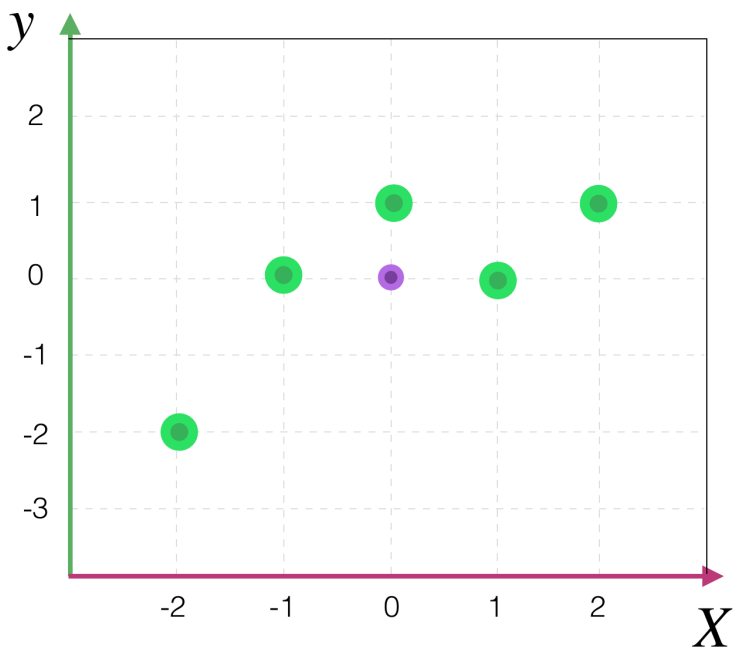
Old coordinate system



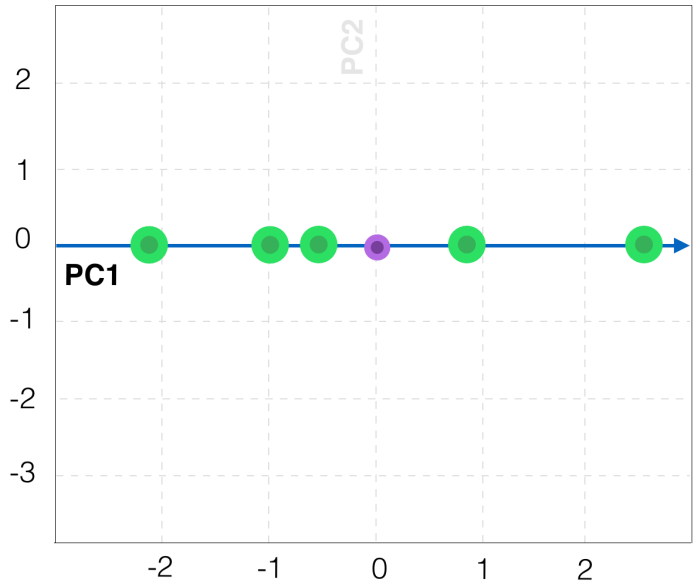
New coordinate system

Principal Component Analysis

We can **ignore** the **second eigenvector**
because it does not contain much information



Old coordinate system

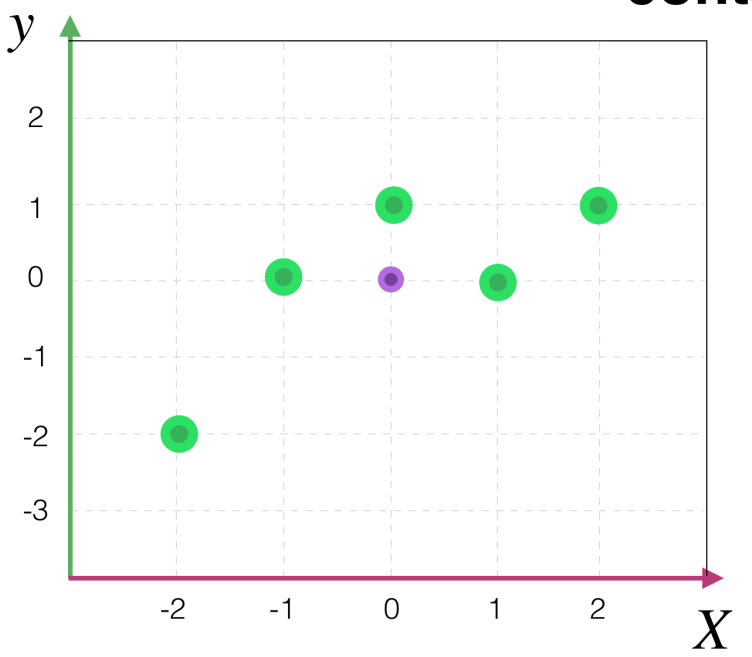


New coordinate system

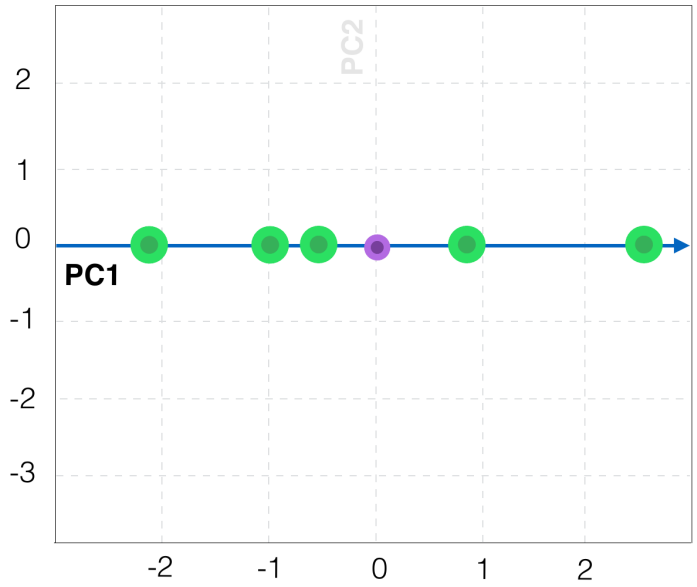
Principal Component Analysis

We can **ignore** the **second eigenvector** because it does not contain much information

How much information **the second eigenvector contains**?

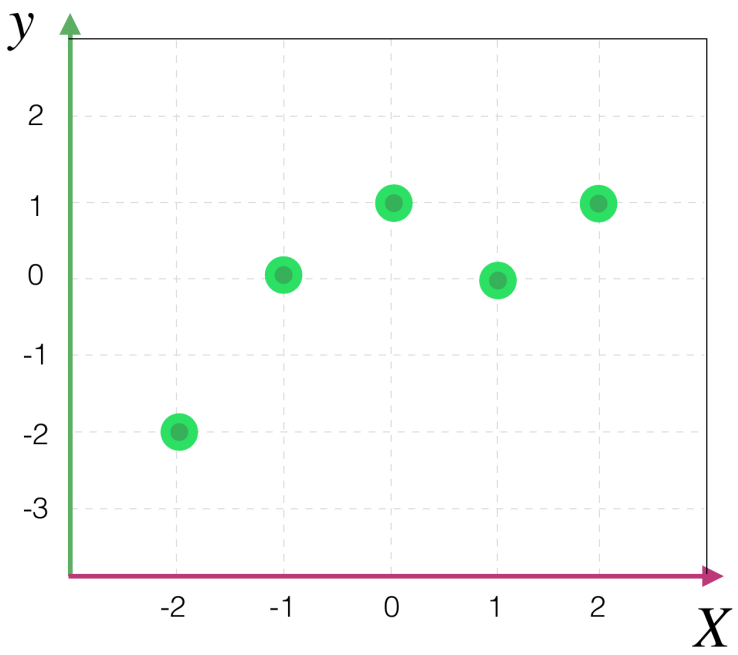


Old coordinate system

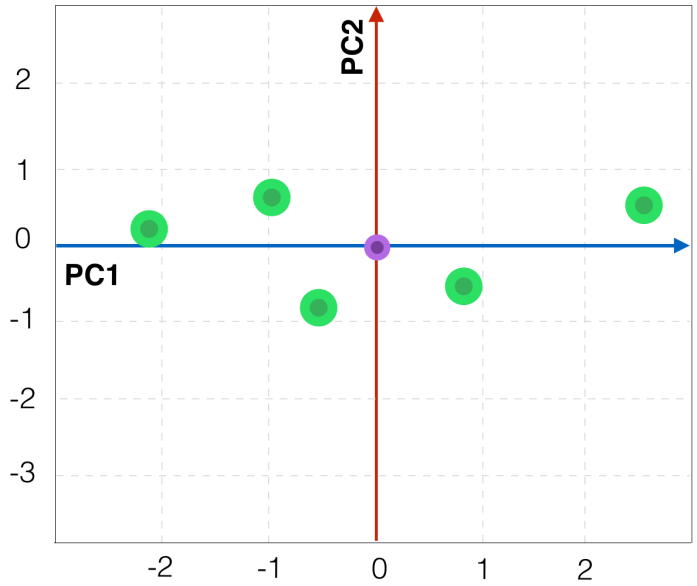


New coordinate system

Principal Component Analysis



Old coordinate system



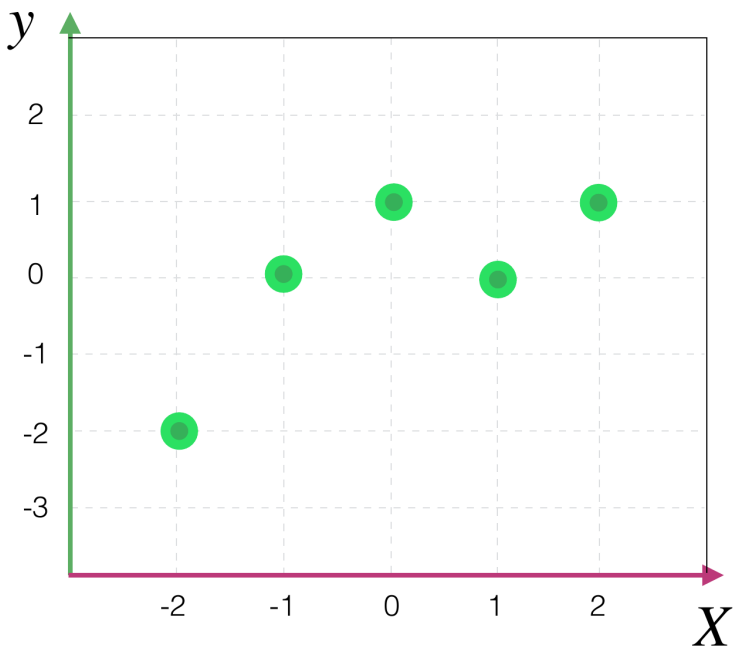
New coordinate system

Principal Component Analysis

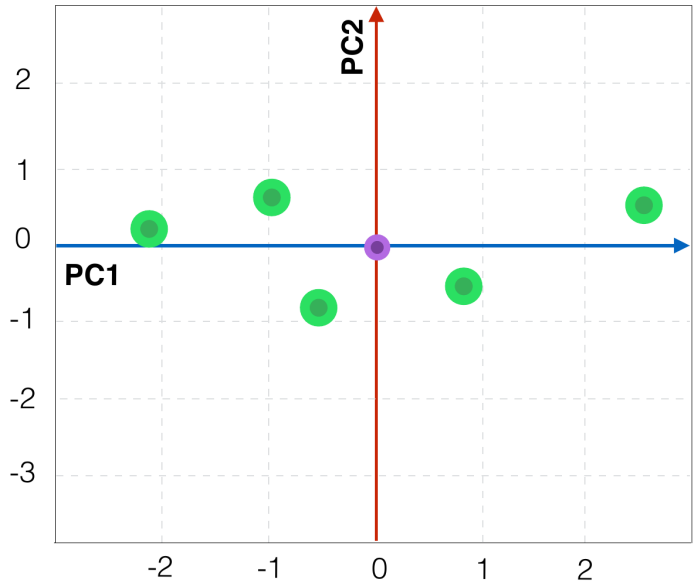
D

3.58	0
0	0.42

Eigen**values**



Old coordinate system



New coordinate system

Principal Component Analysis

S

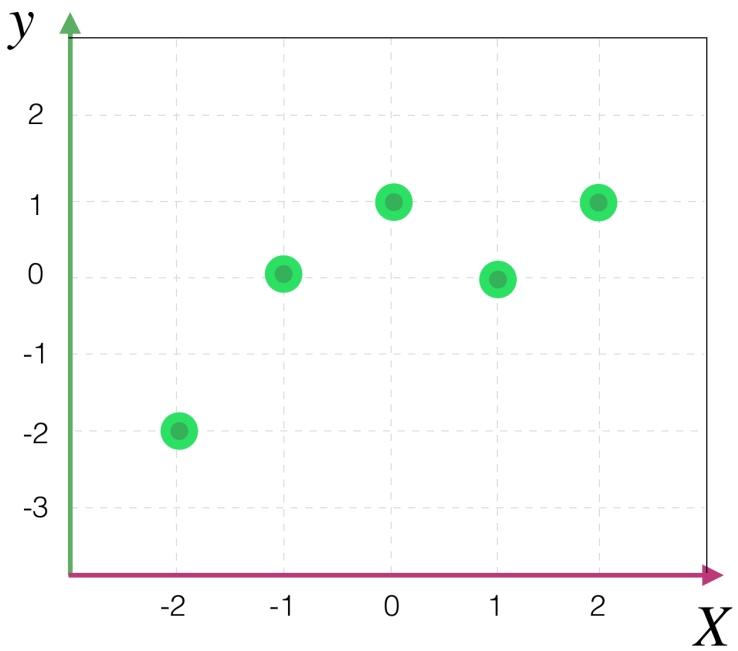
2.5	1.5
1.5	1.5

Covariance matrix

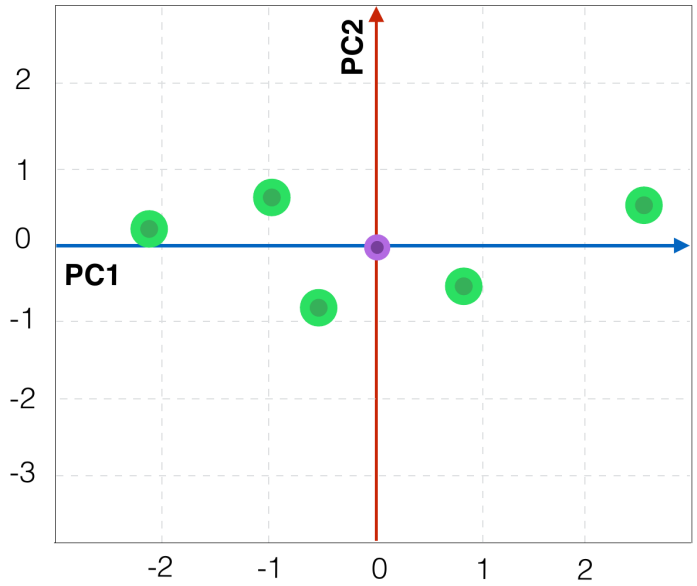
D

3.58	0
0	0.42

Eigen**values**

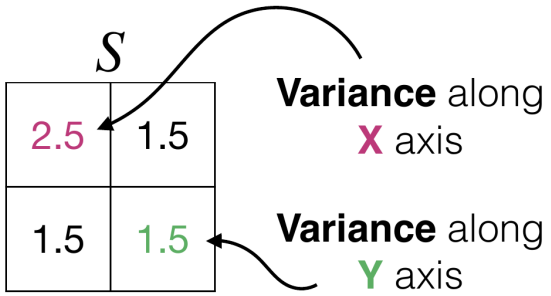


Old coordinate system



New coordinate system

Principal Component Analysis

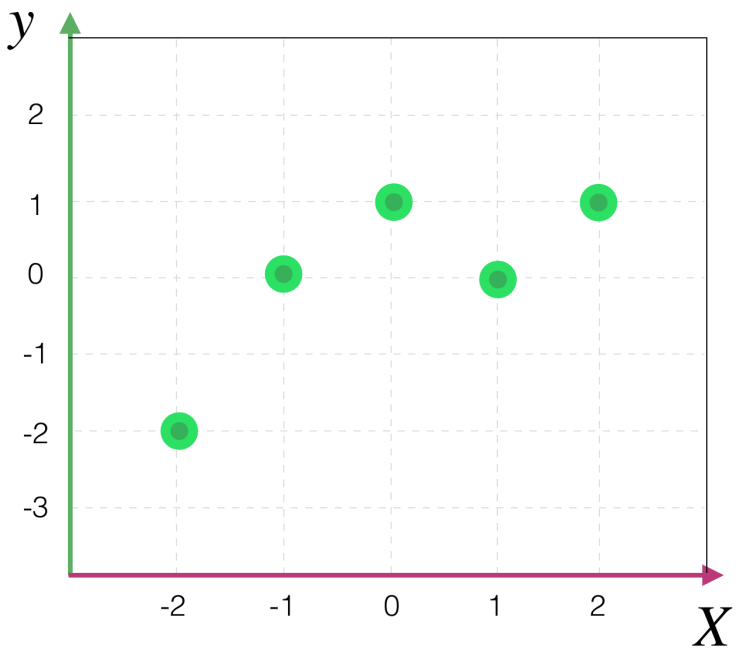


Covariance matrix

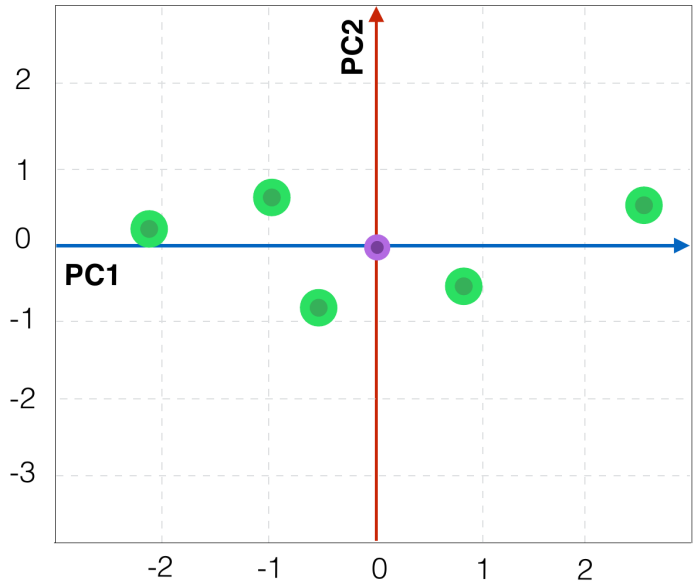
D

3.58	0
0	0.42

Eigen**values**

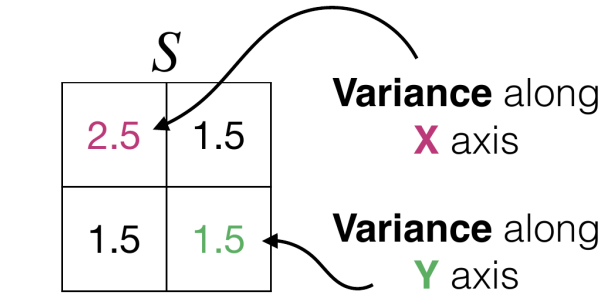


Old coordinate system



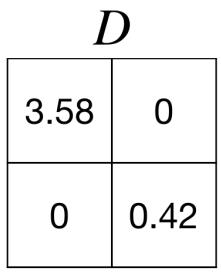
New coordinate system

Principal Component Analysis



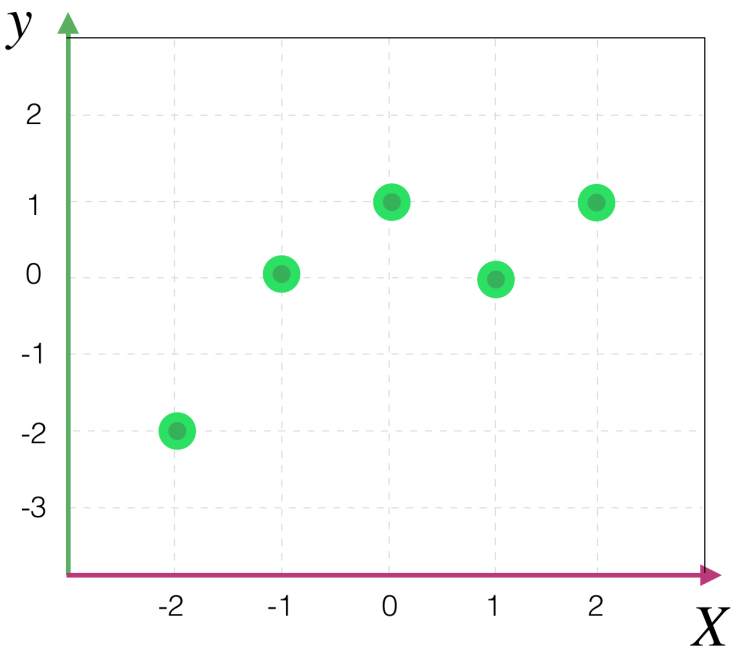
Covariance matrix

Variance along **?**

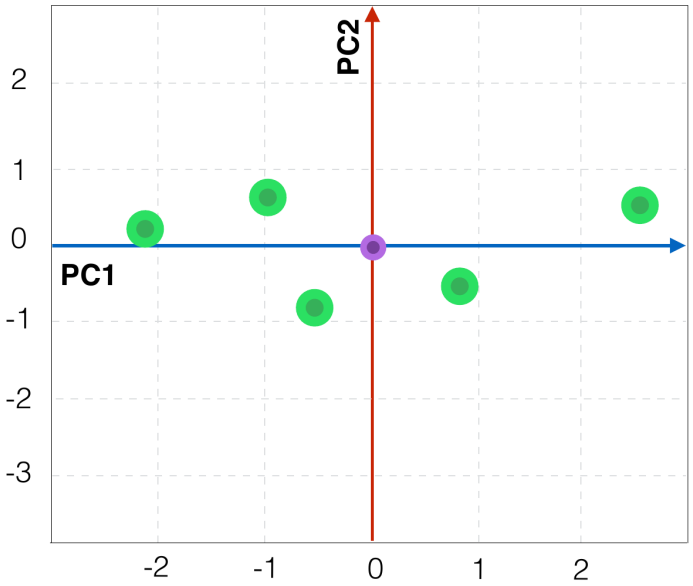


Variance along **?**

Eigen**values**

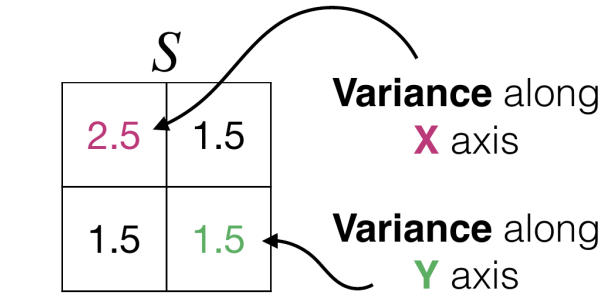


Old coordinate system



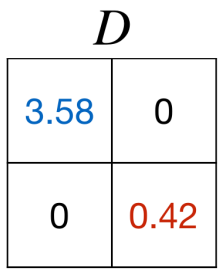
New coordinate system

Principal Component Analysis



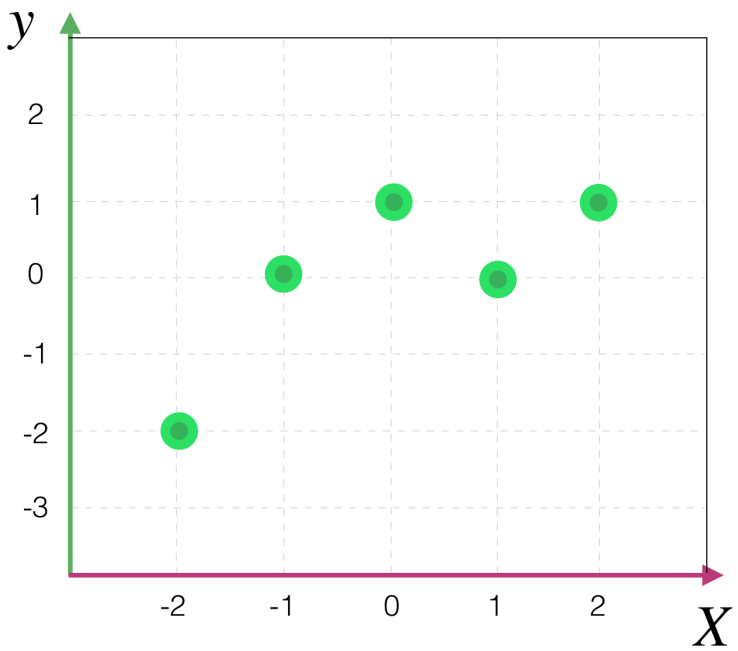
Covariance matrix

Variance along **PC1**

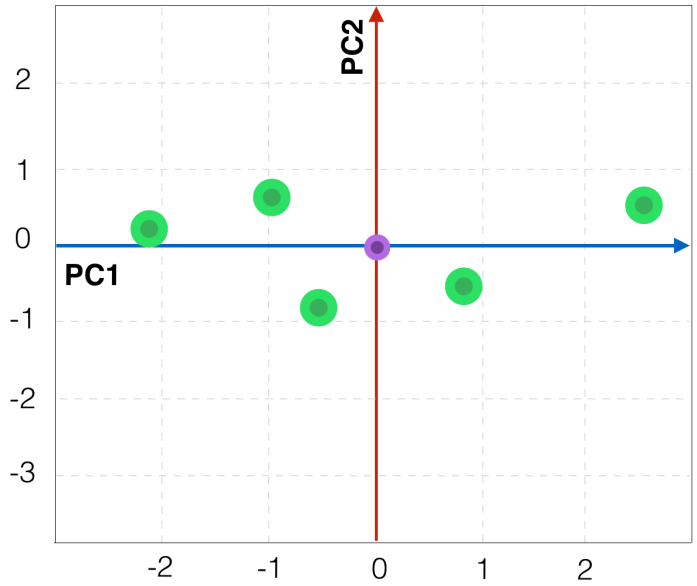


Variance along **PC2**

Eigen**values**

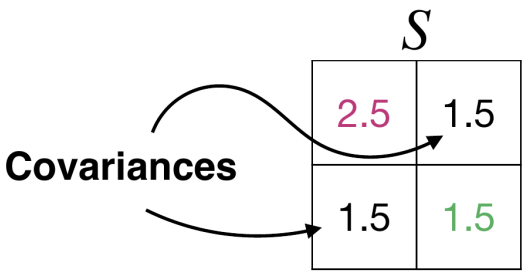


Old coordinate system

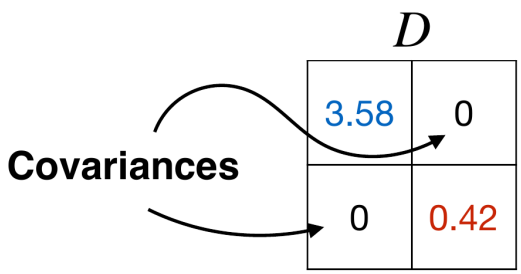


New coordinate system

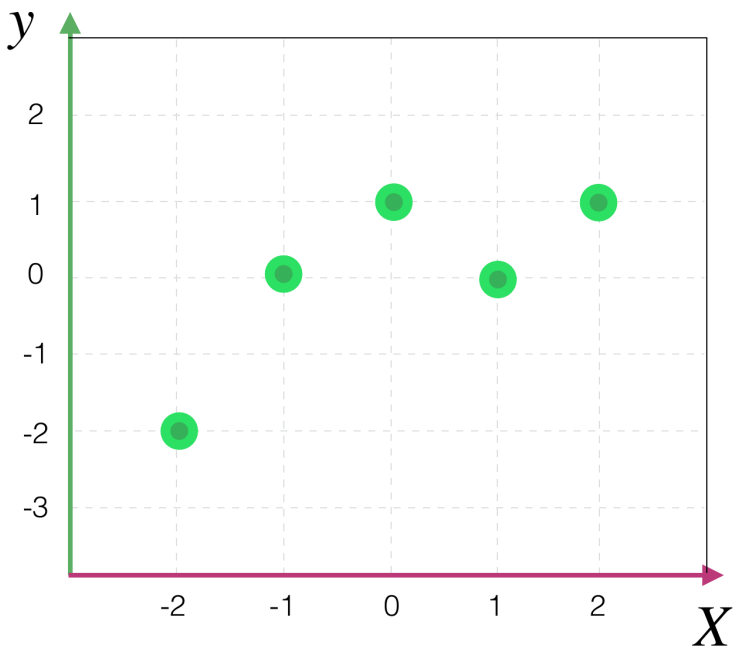
Principal Component Analysis



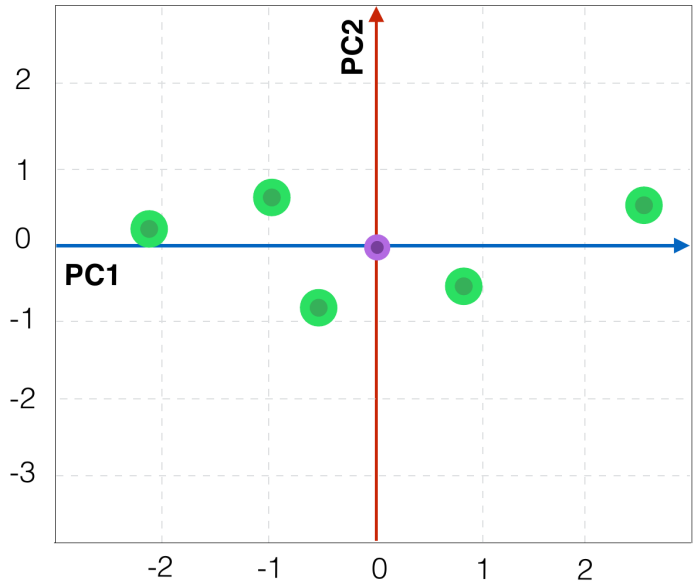
Covariance matrix



Eigen**values**



Old coordinate system



New coordinate system

Principal Component Analysis

S

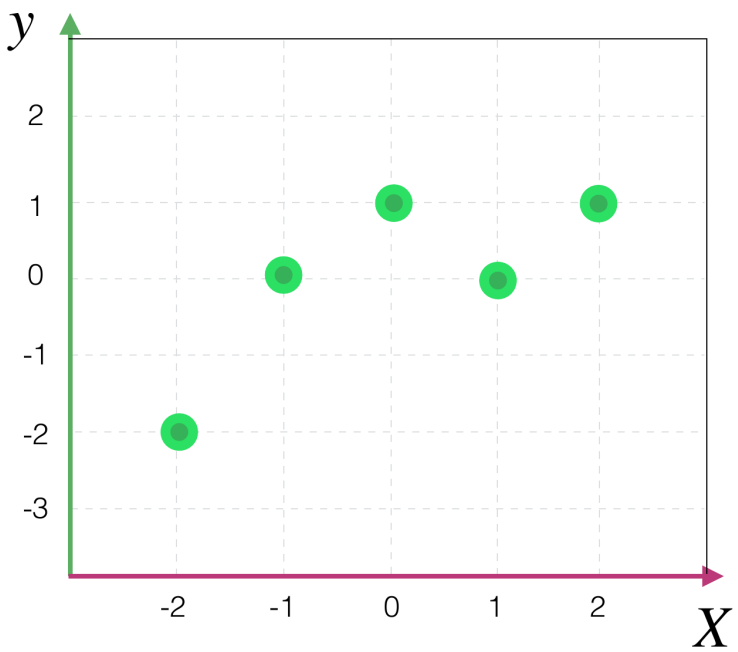
2.5	1.5
1.5	1.5

Covariance matrix

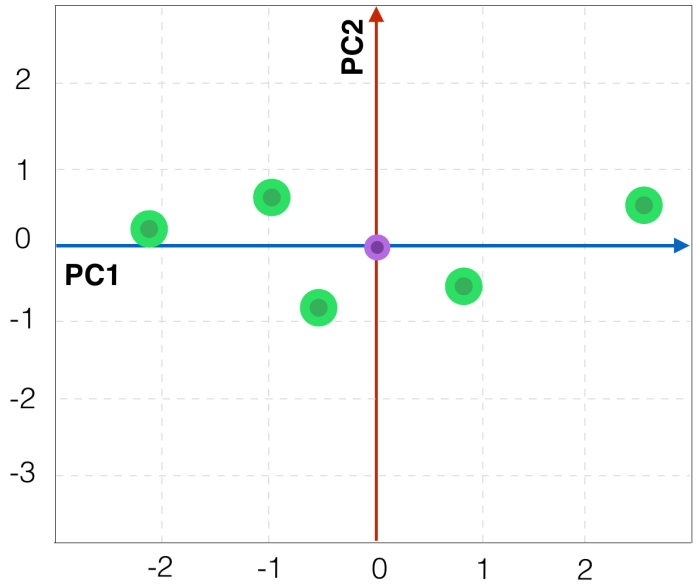
D

3.58	0
0	0.42

New **covariance** matrix



Old coordinate system



New coordinate system

Principal Component Analysis

S

2.5	1.5
1.5	1.5

Covariance matrix

D

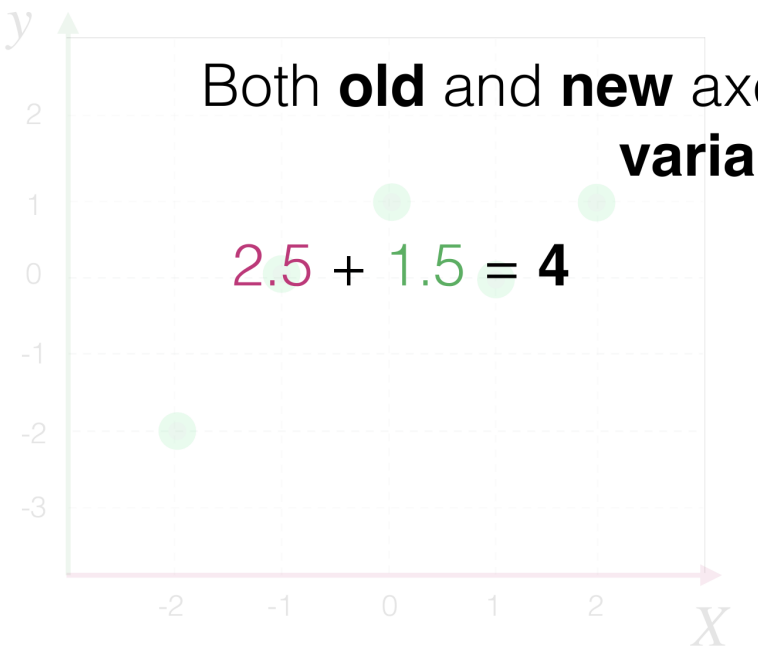
3.58	0
0	0.42

New **covariance** matrix

Both **old** and **new** axes explain **4** units of **variance**

$2.5 + 1.5 = \mathbf{4}$

$3.58 + 0.42 = \mathbf{4}$



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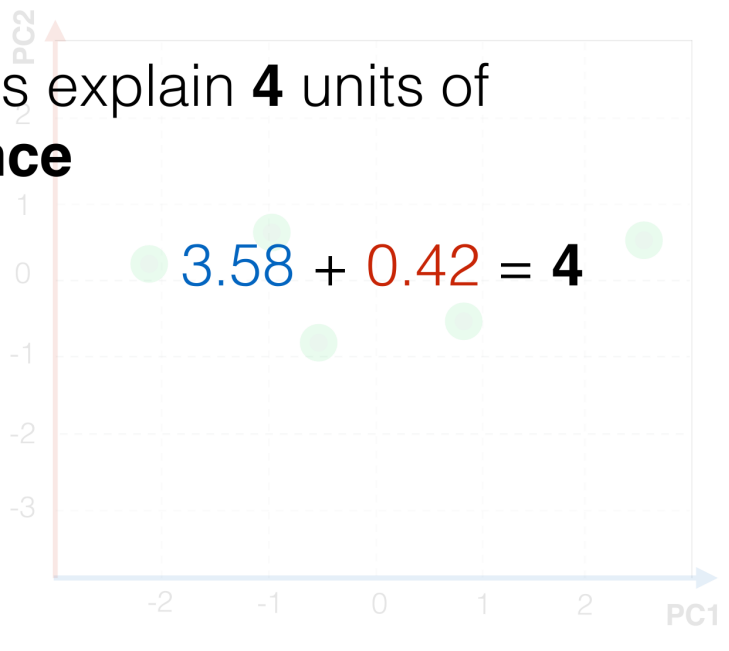

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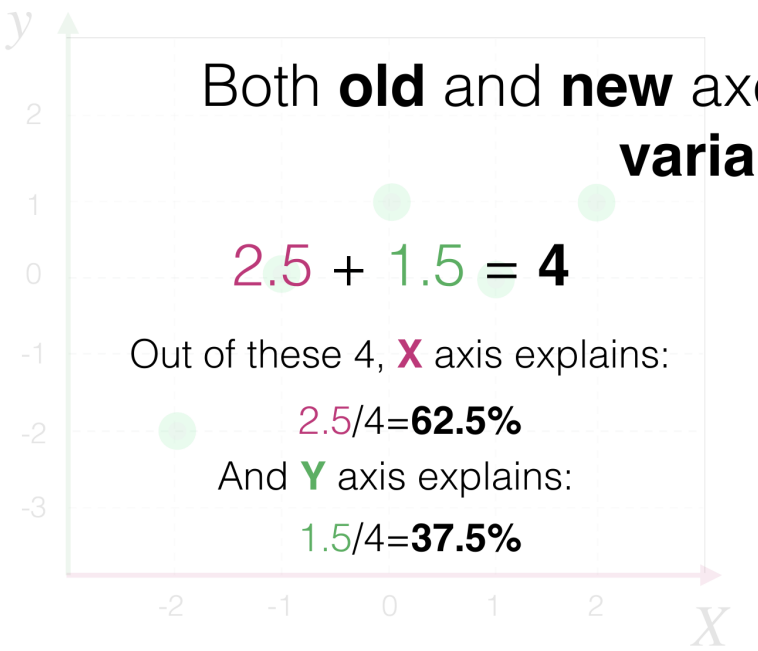
Out of these 4, **X** axis explains:

2.5/4=**62.5%**

And **Y** axis explains:

1.5/4=**37.5%**



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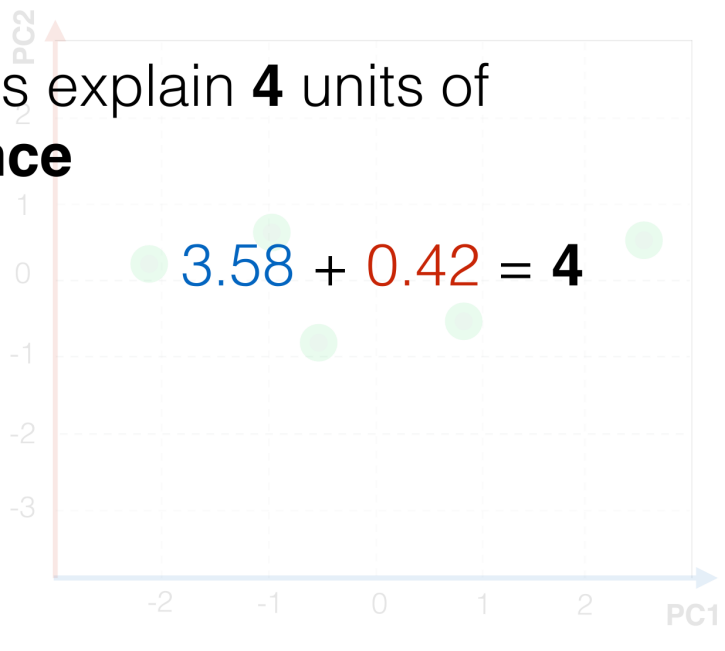

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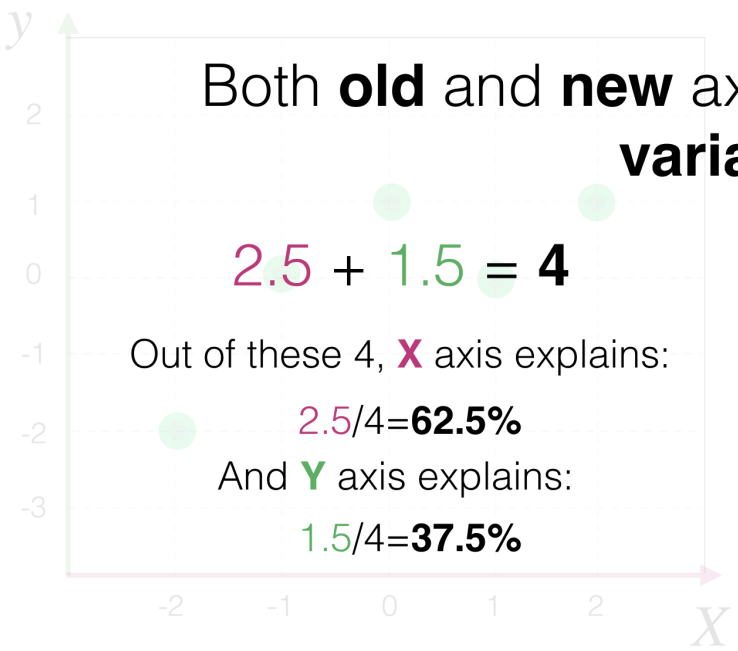


Old coordinate system

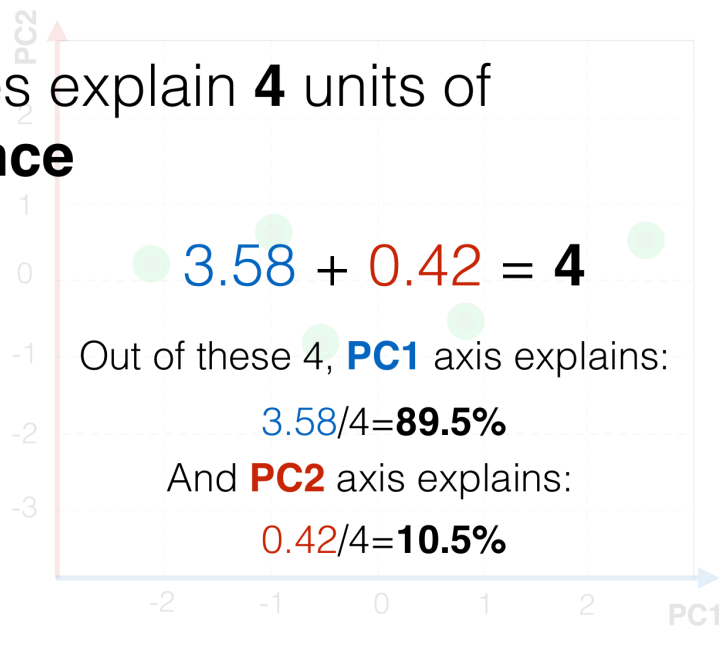
3.58 + 0.42 = **4**

Out of these 4, **PC1** axis explains:

3.58/4=**89.5%**

And **PC2** axis explains:

0.42/4=**10.5%**

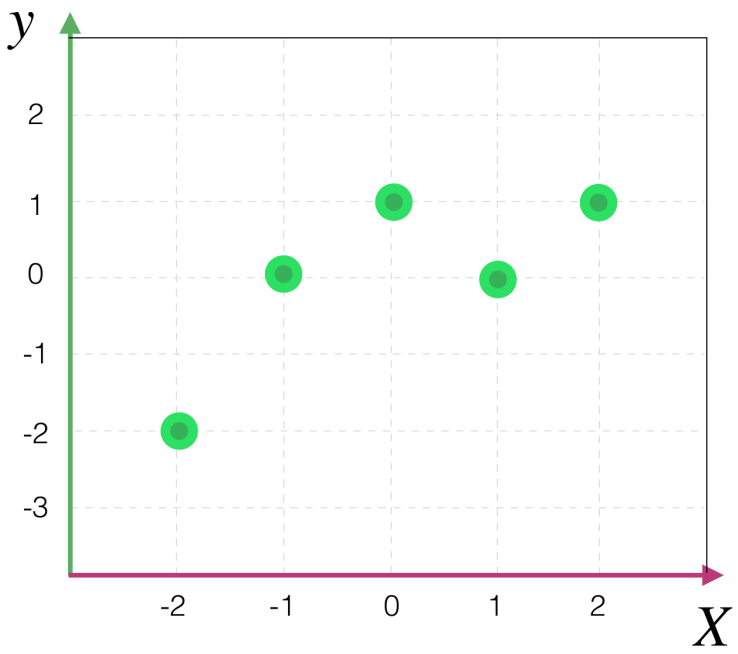


New coordinate system

Principal Component Analysis

We can **ignore** the **second PC** because it does not contain much information

How much information **the second PC contains**?



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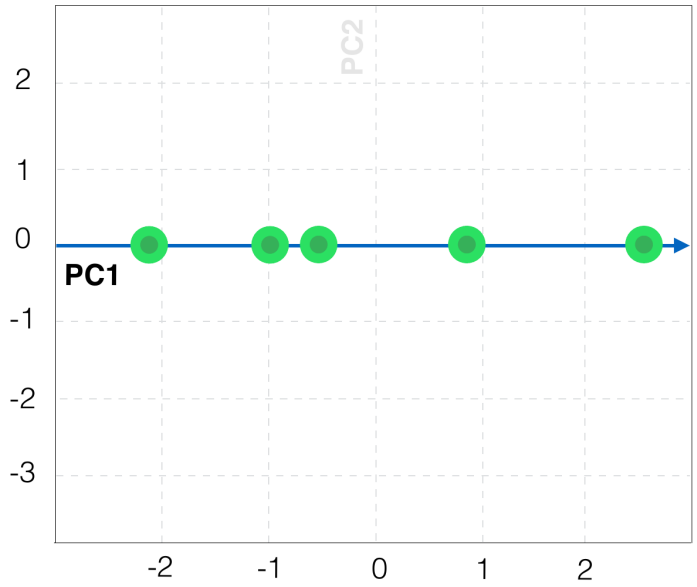
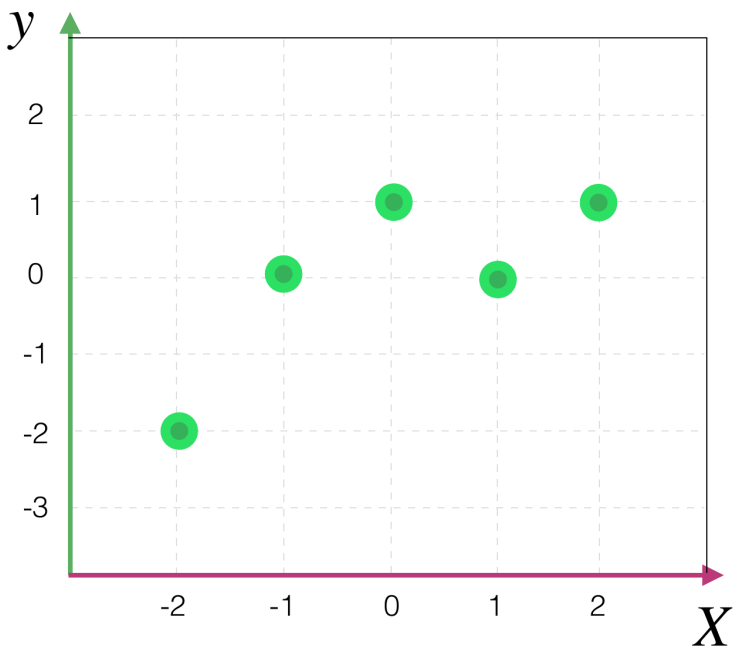


New coordinate system

Principal Component Analysis

We can **ignore** the **second PC** because it explains only **10.5%** of variation



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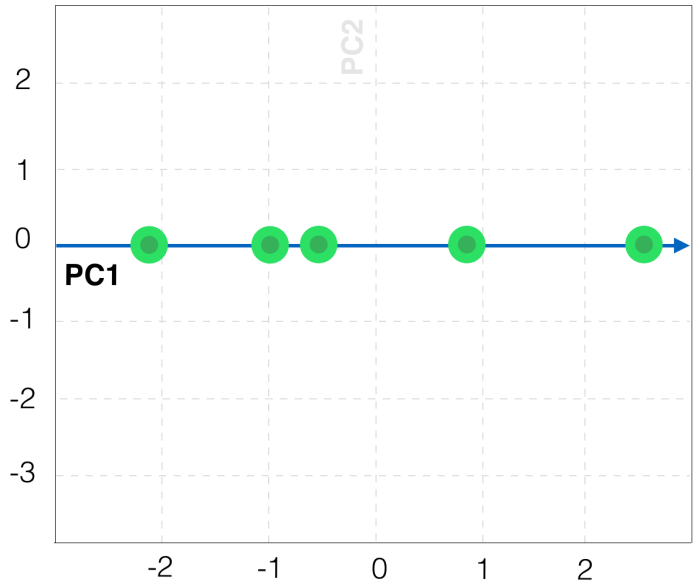
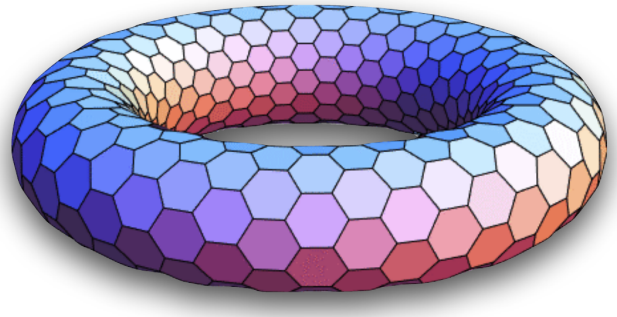
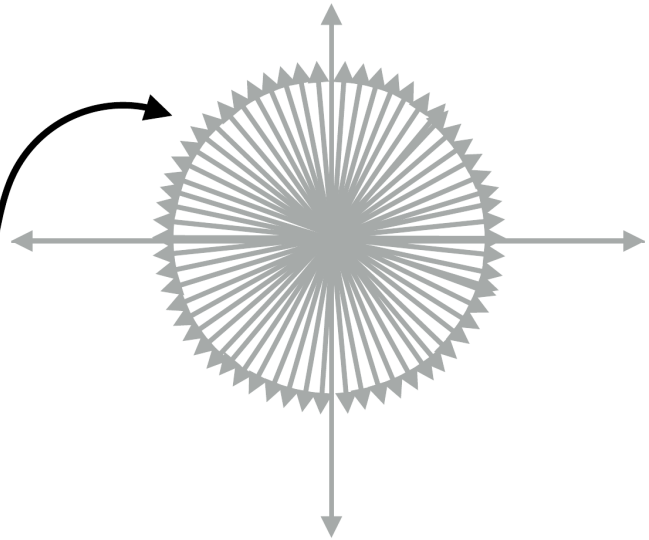


New coordinate system

Principal Component Analysis

How many PCs will be formed in **200D** space?





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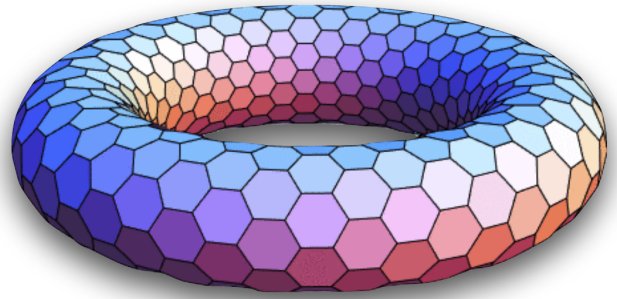

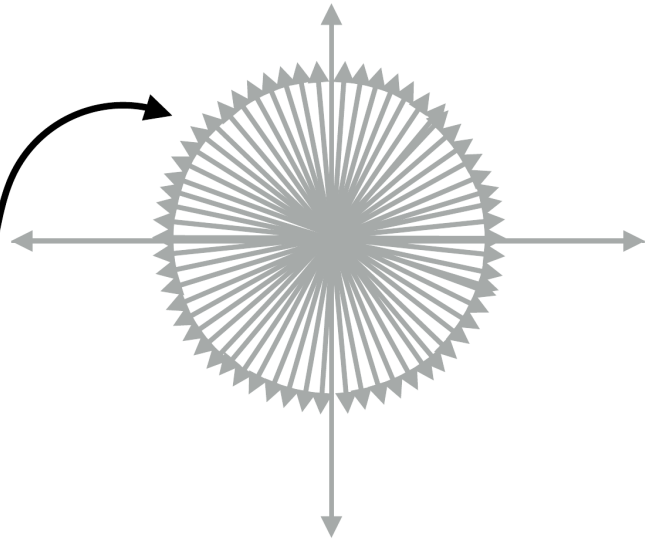

No exceptions, **200 PCs**

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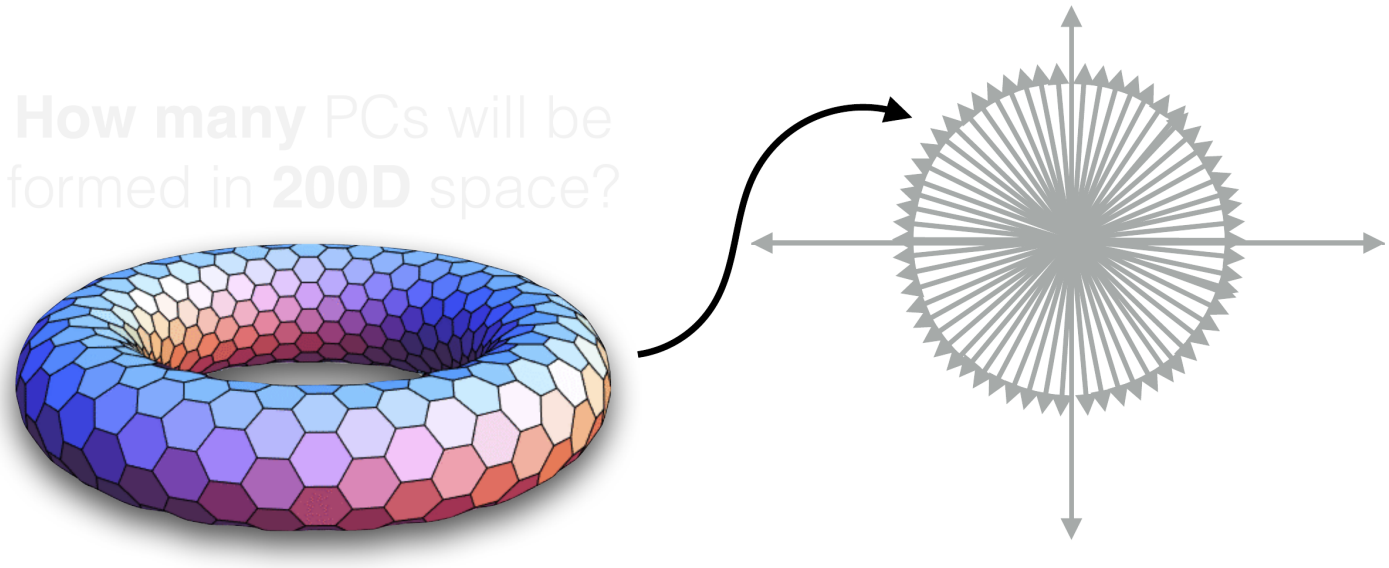

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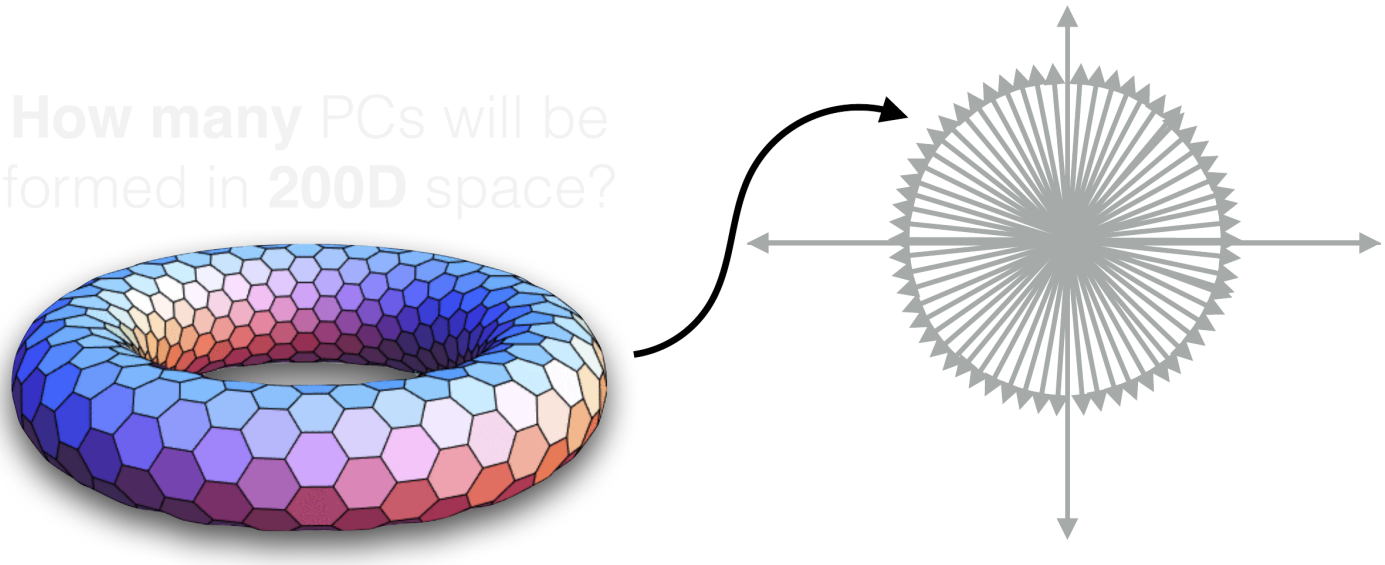
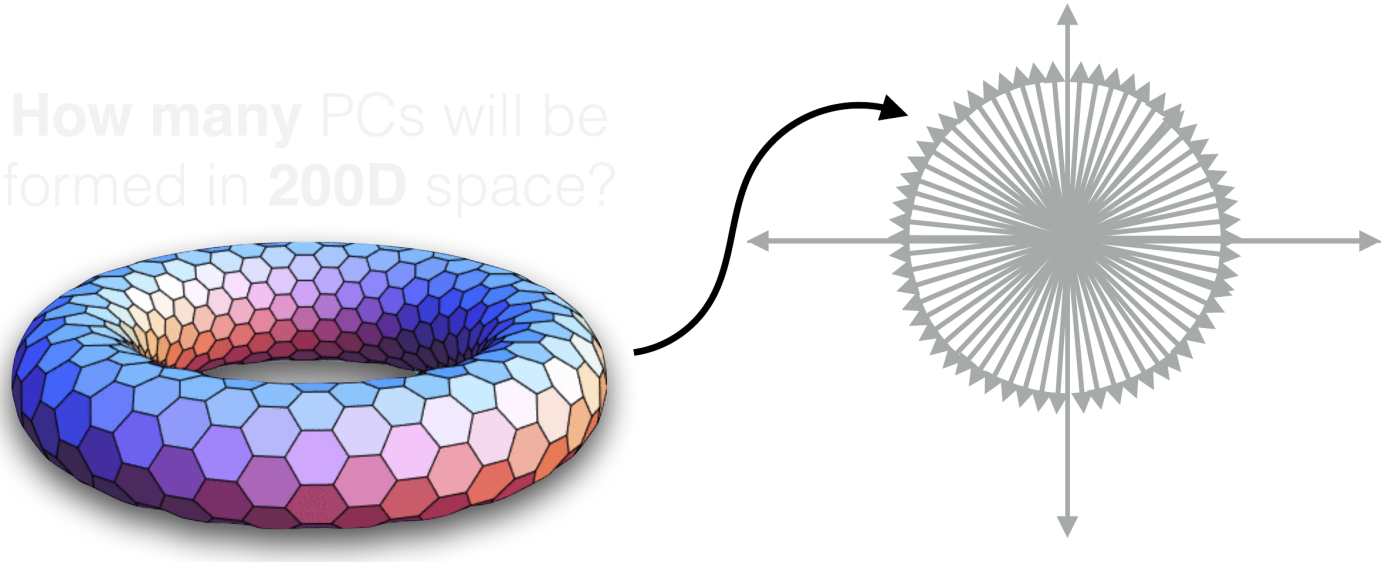


How many PCs should we keep?

Principal Component Analysis

Variance explained is a good criteria for choosing the total number of PCs to keep



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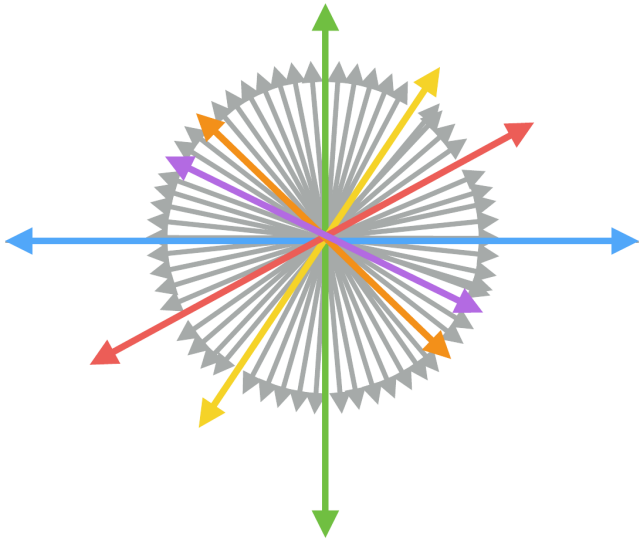

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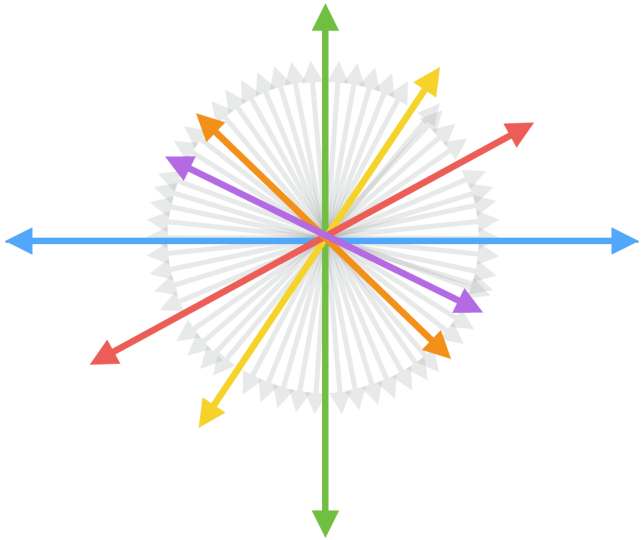

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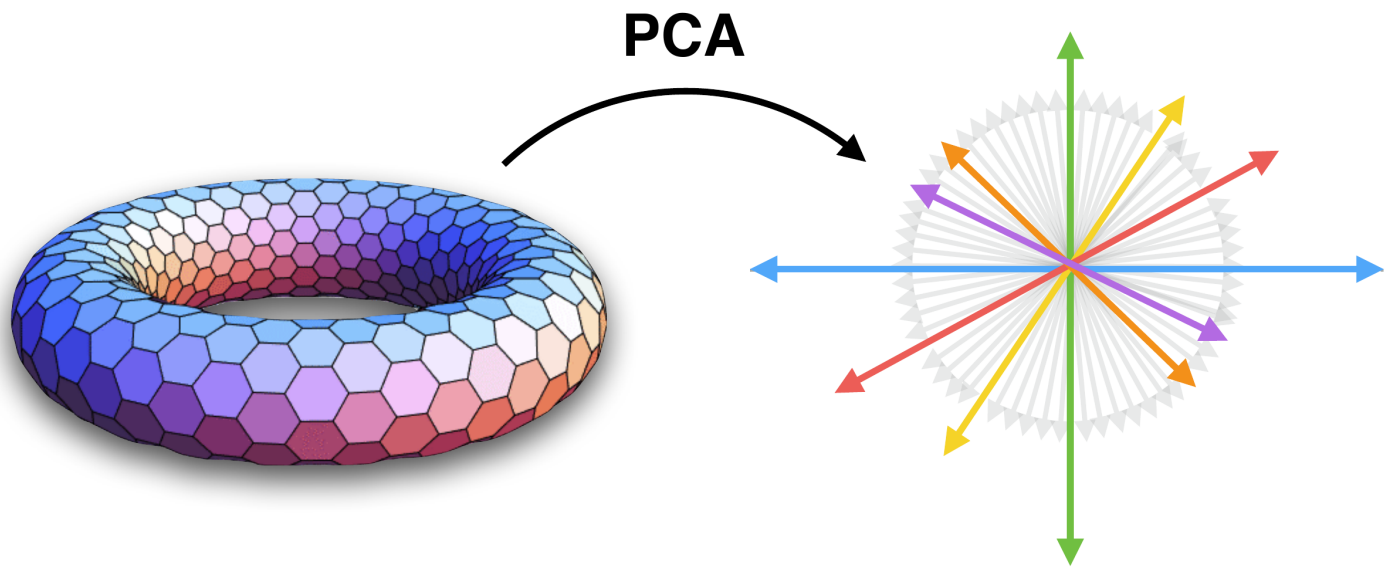
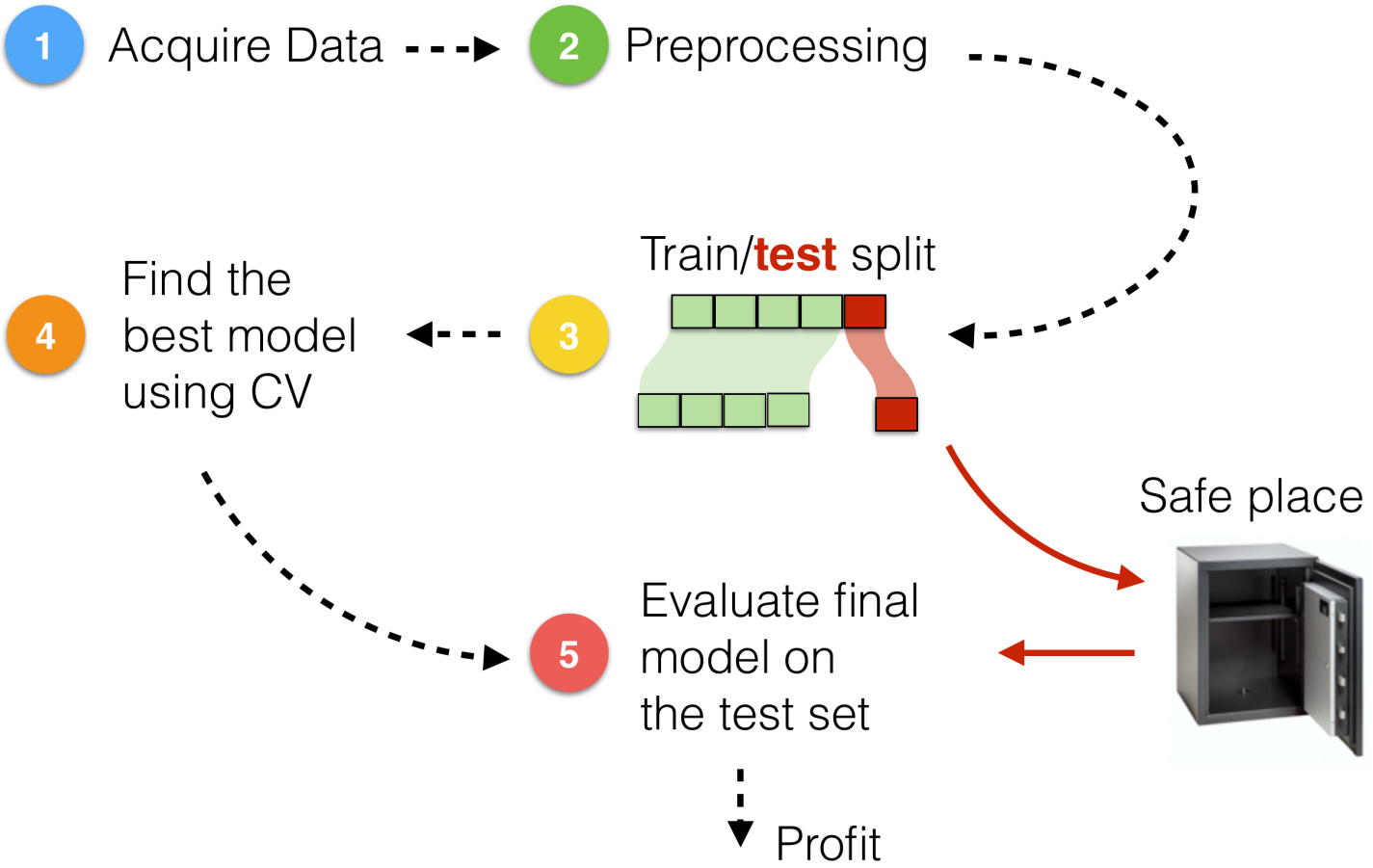
Principle Component Analysis (**PCA**)



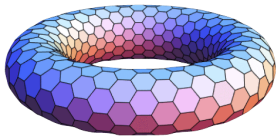
Can be used as part of supervised learning pipeline

Supervised Learning pipeline



Supervised Learning pipeline

1



200D raw data

2 Preprocessing

Train/**test** split

3

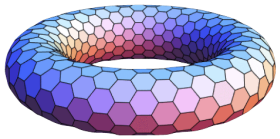
4 Find the best model using CV

Safe place

5 Evaluate final model on the test set

Profit

Supervised Learning pipeline

1  ---▸ 2 Normalisation (subtract mean)

200D raw data

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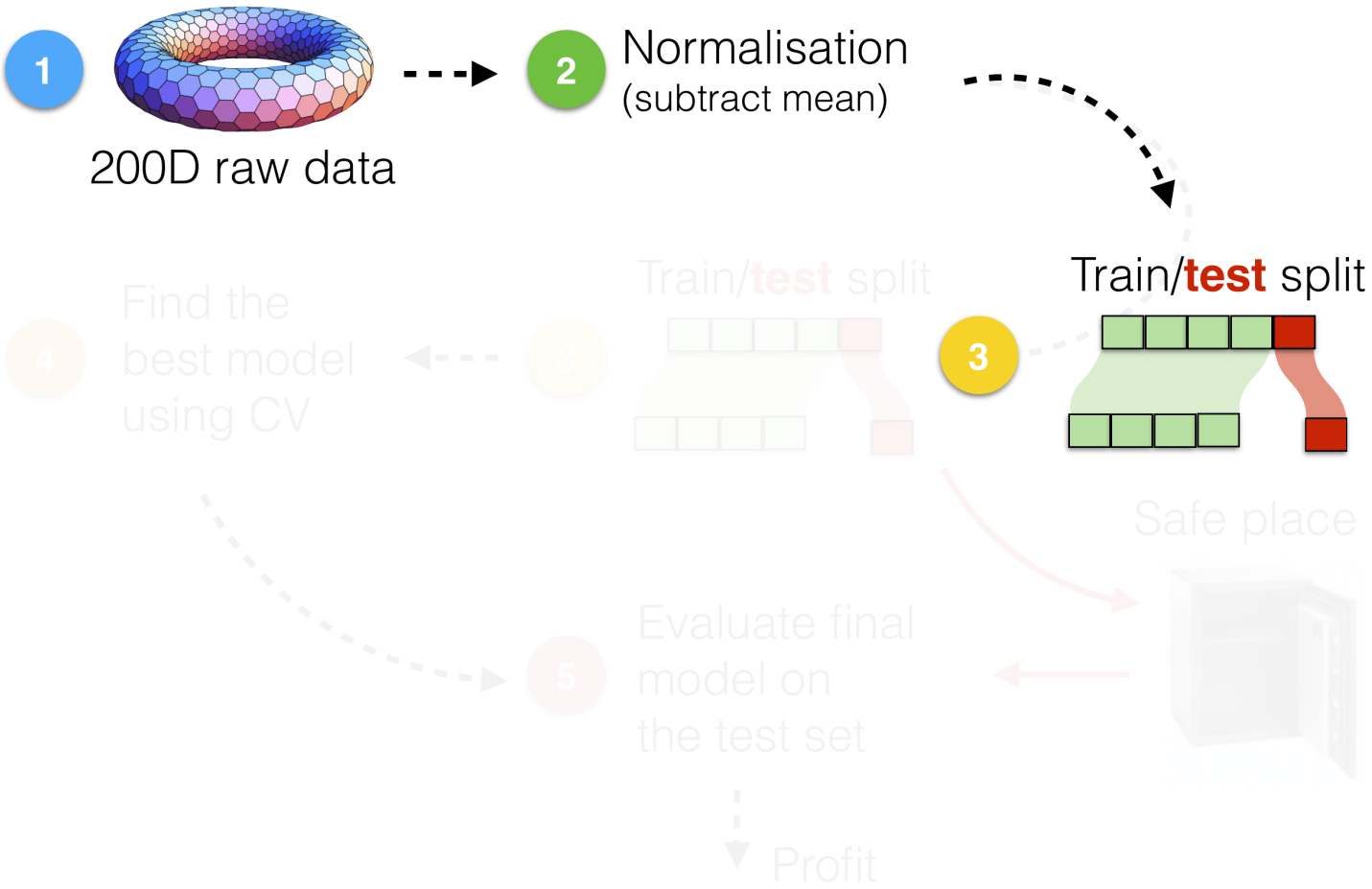
Supervised Learning pipeline



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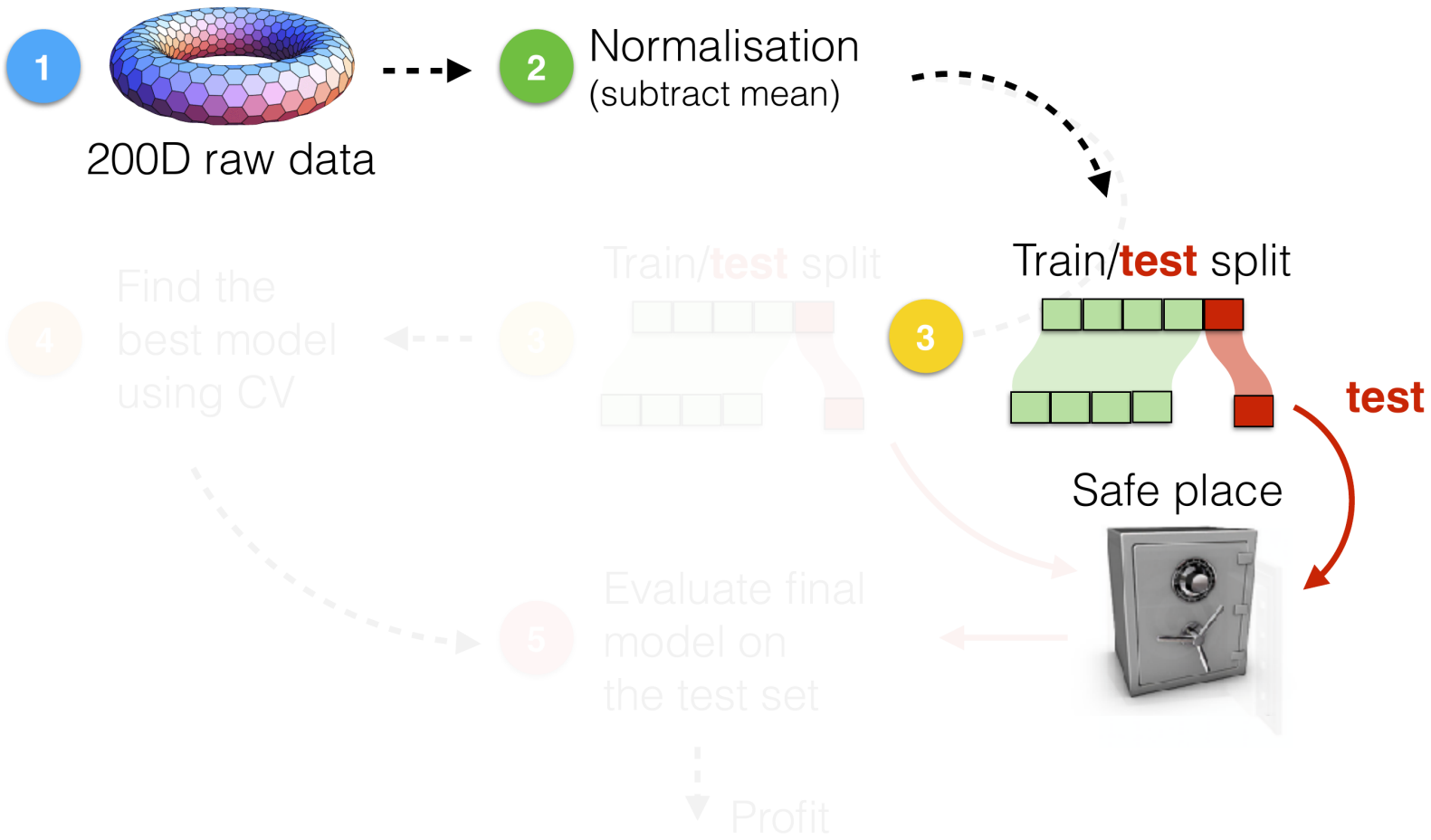

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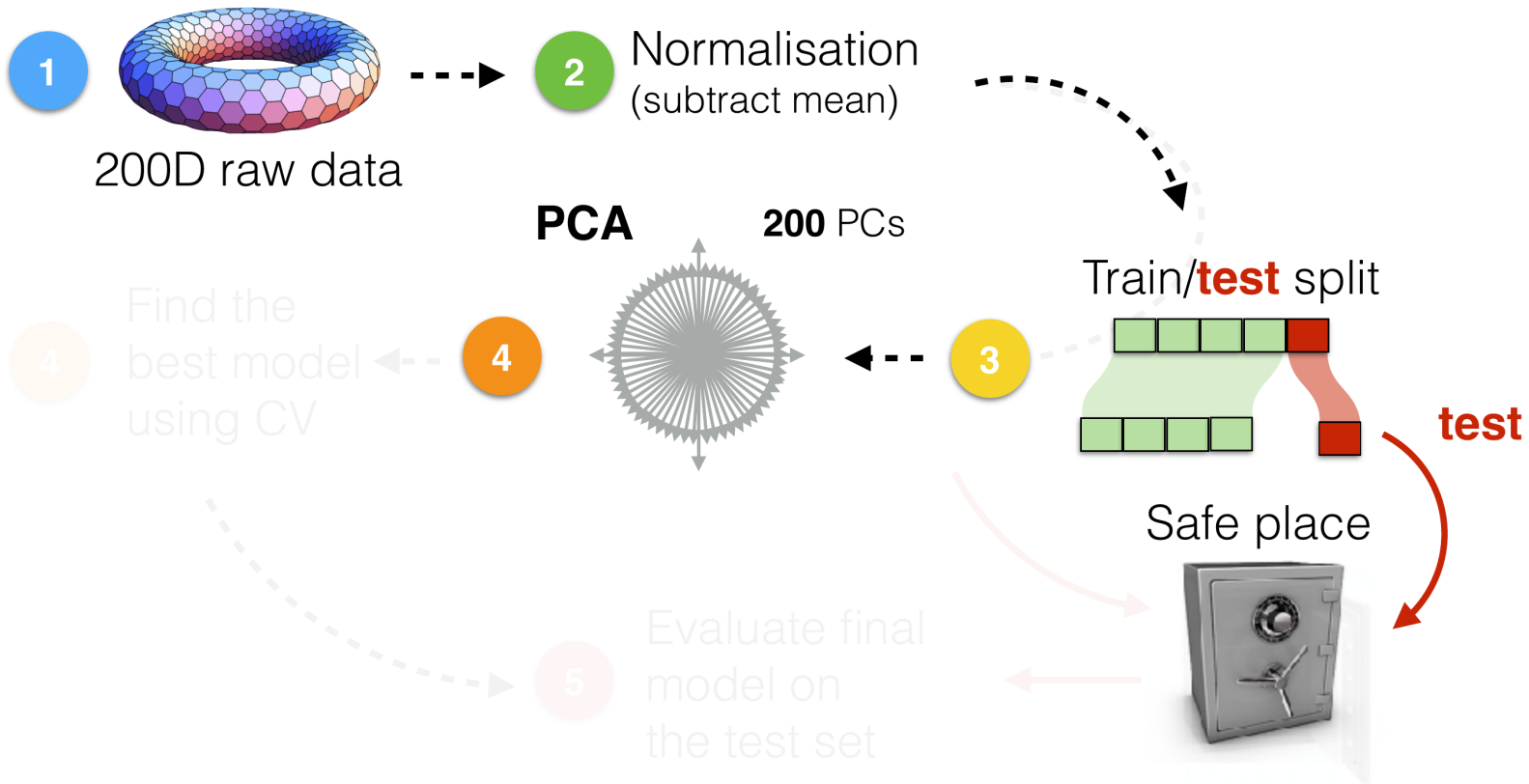

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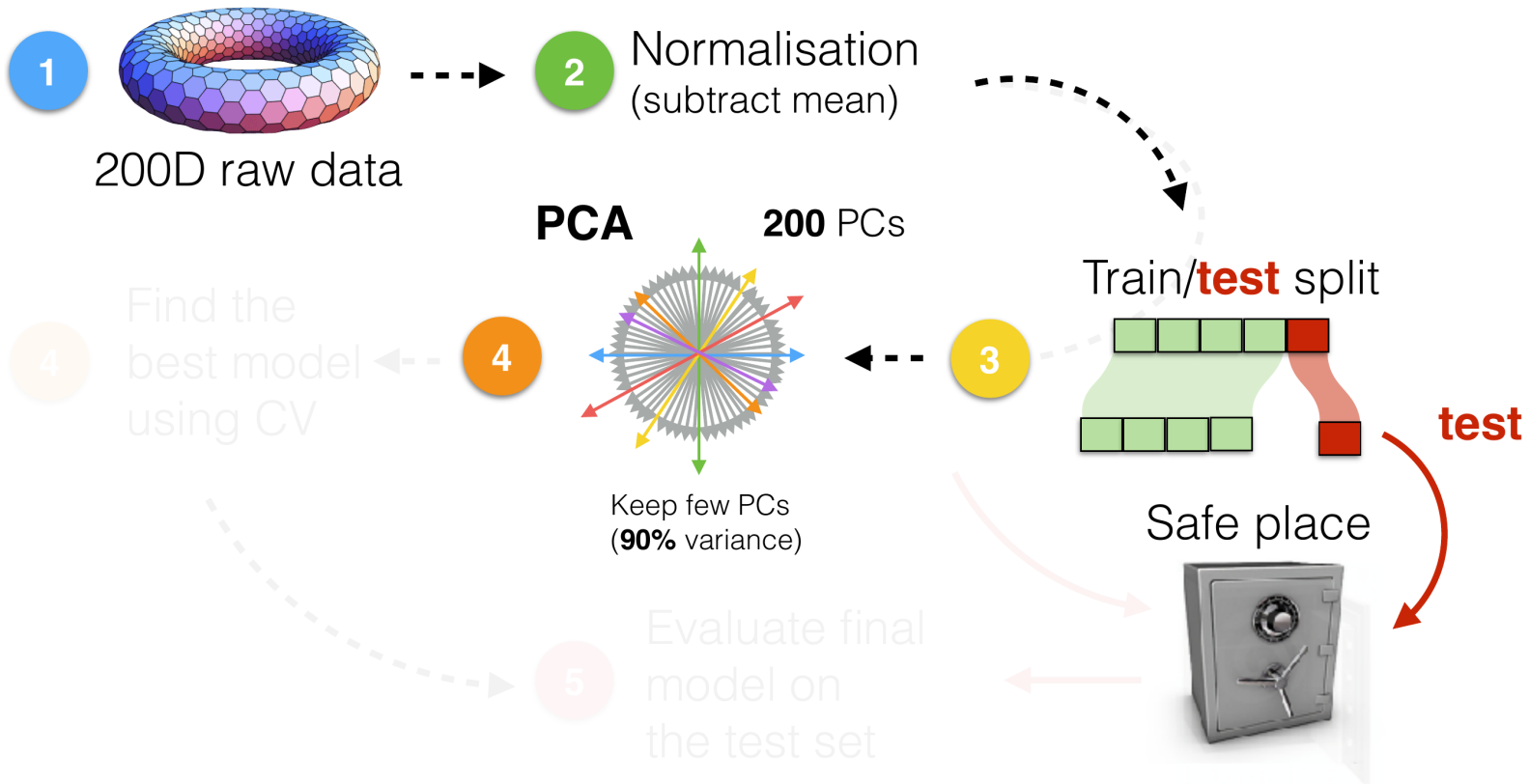

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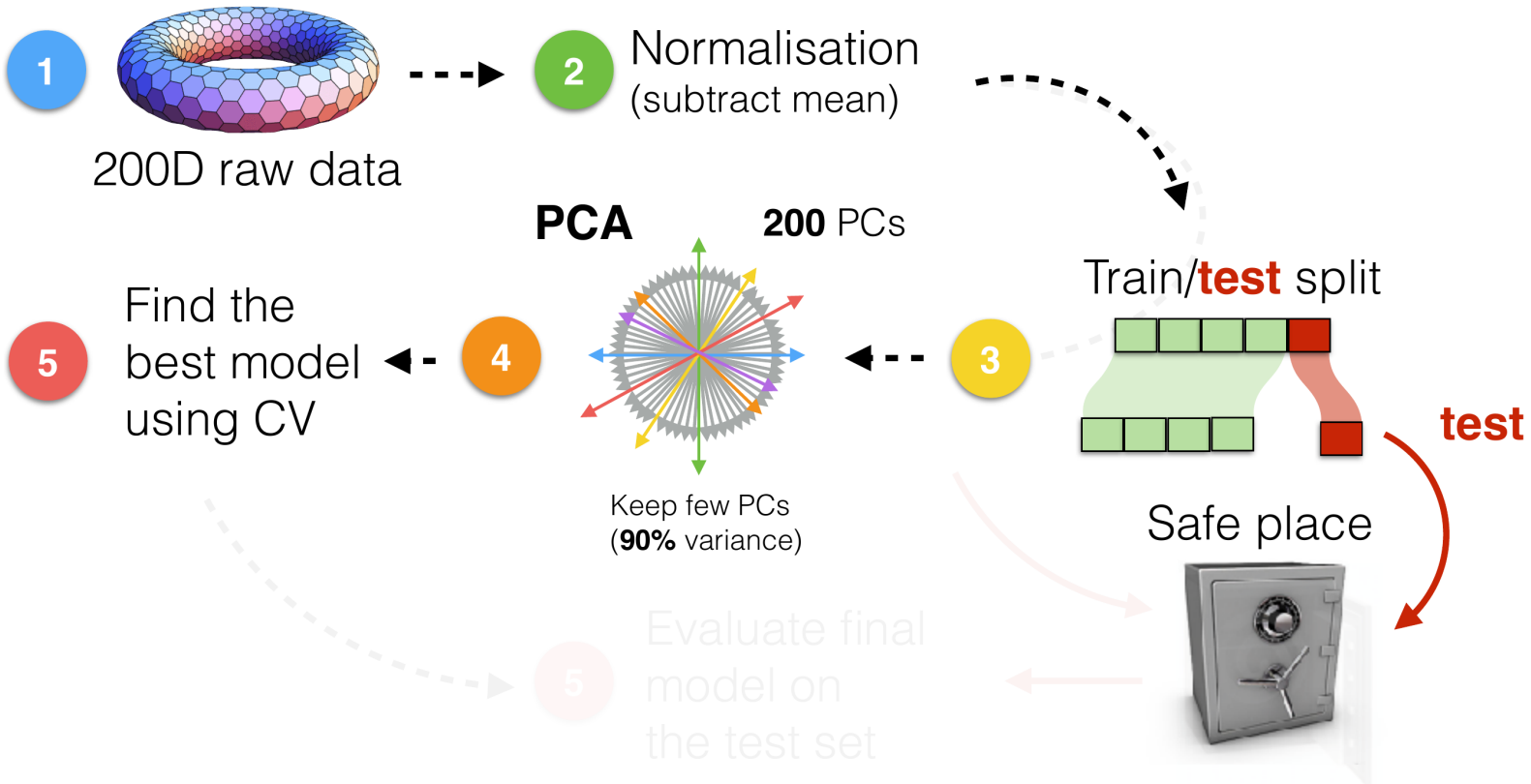

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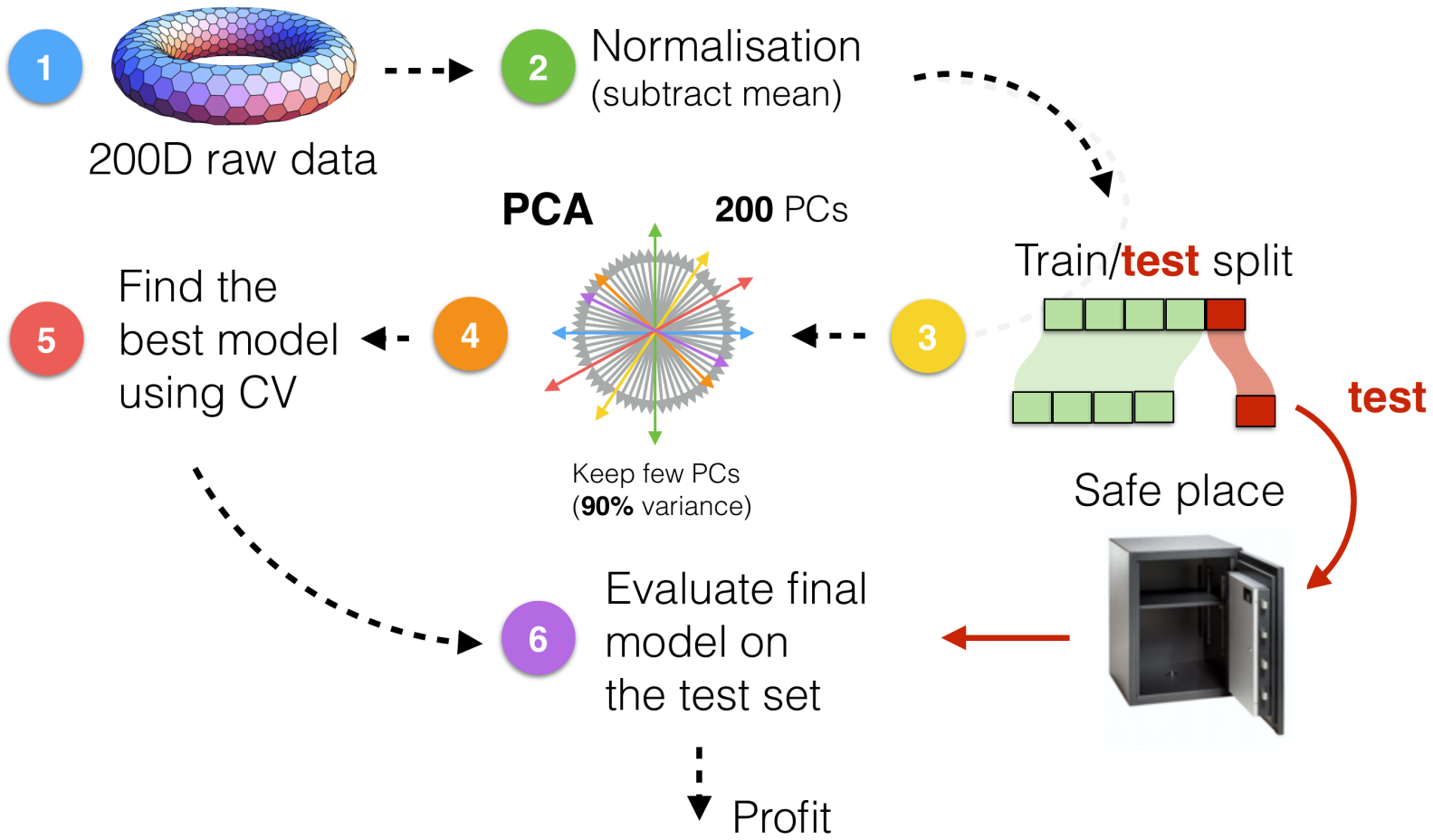
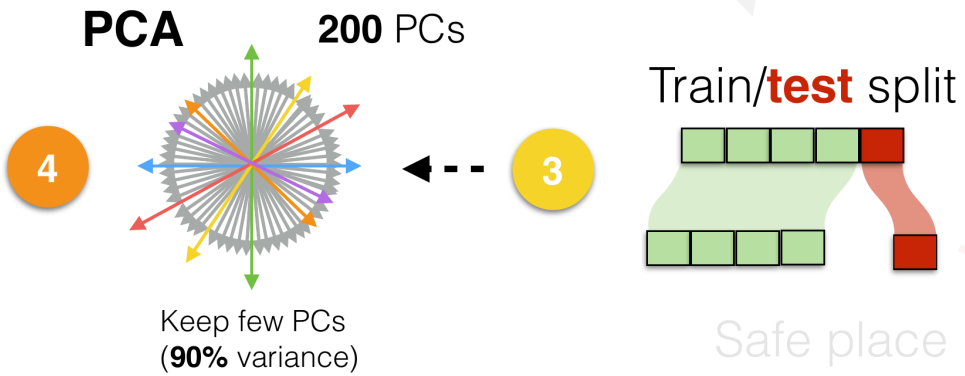


Supervised Learning pipeline

Here, **PCA** is performed only on **training data**



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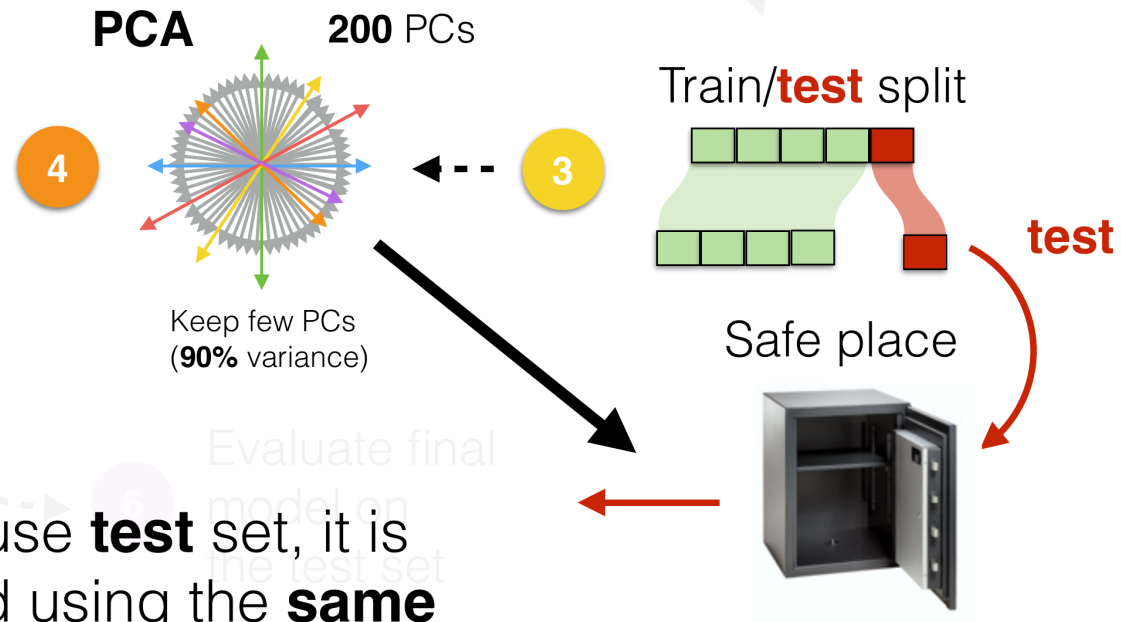
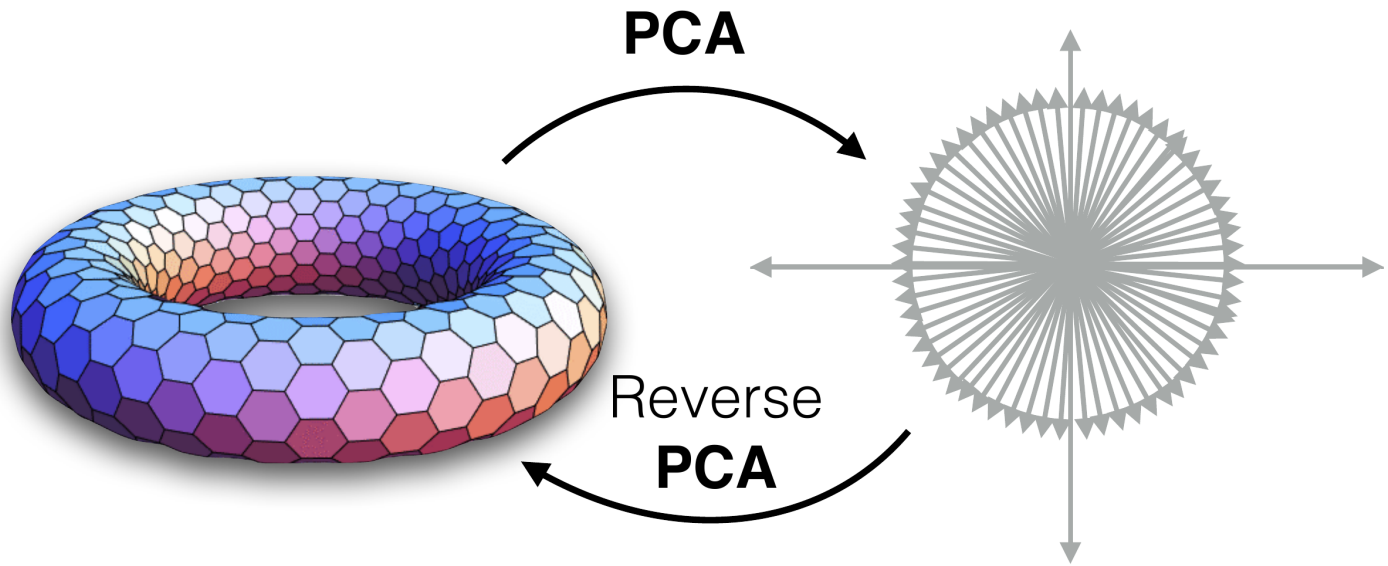


When we use **test** set, it is transformed using the **same eigenvectors** as **training** data

Principal Component Analysis

PCA has an "**undo**" button



You can **recover** the **original features** back!

PCA has an "**undo**" button

Conventional PCA

$$eigenvectors \times Z^{\top}_{original} = Z_{transformed}$$

Reversed PCA

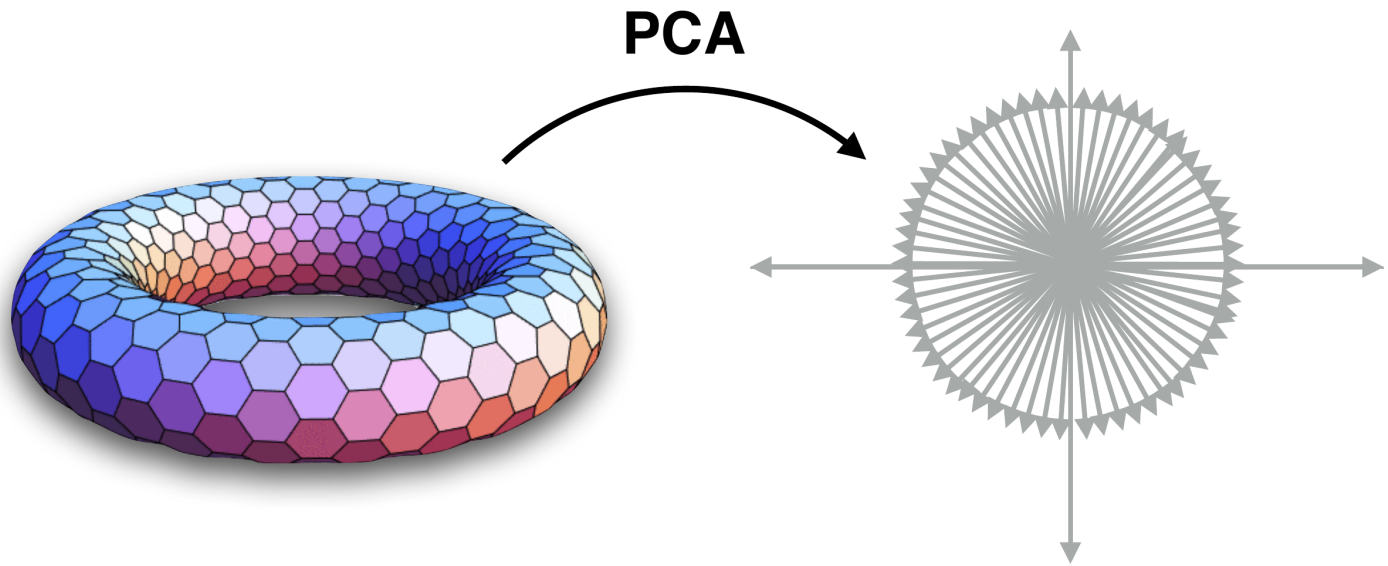
$$eigenvectors^{\top} \times Z_{transformed} = Z_{original}$$

You can **recover** the **original features** back!

Convince yourself: http://www.cs.otago.ac.nz/cosc453/student_tutorials/principal_components.pdf

Principal Component Analysis

Principle components **are linear combinations** of **original features**



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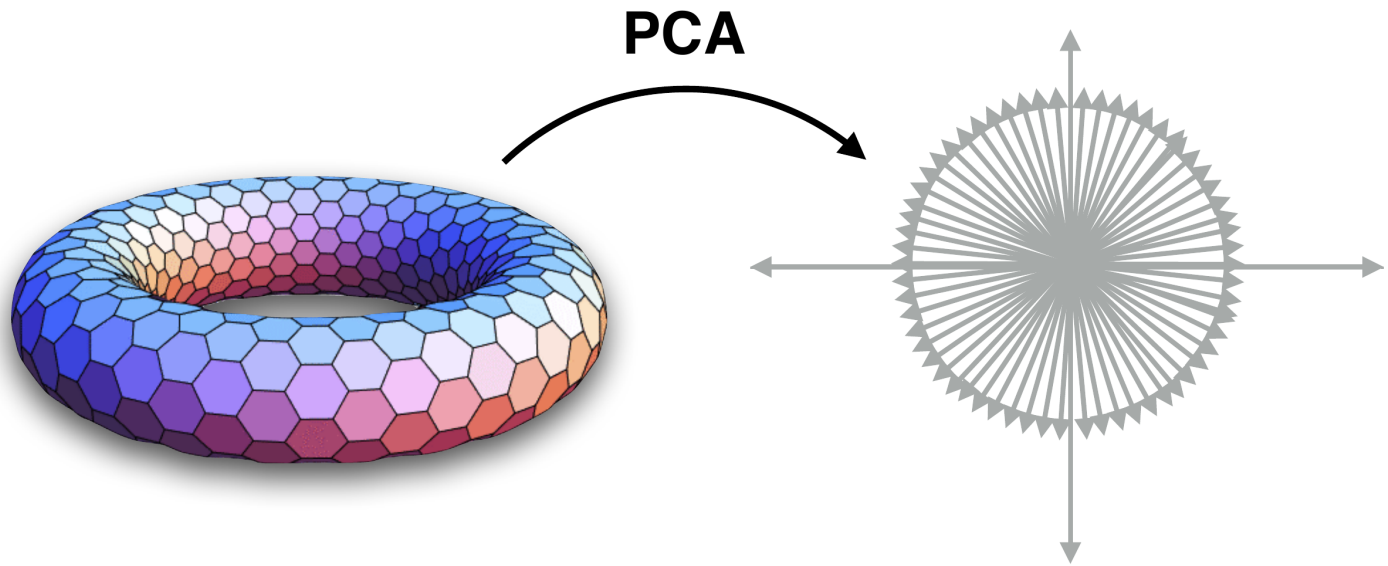

So if you predict anything based on PCs, the **meaning** of original features **is not preserved** after the transformation

Problem Setting of PCA

- In PCA, we are interested in finding projections $\mathbf{x}'_n$ of data points $\mathbf{x}_n$ that are as similar to the original data points as possible, but which have a significantly lower intrinsic dimensionality.

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$$\mathbf{z}_n = \mathbf{B}^T\mathbf{x}_n \in \mathbb{R}^M,$$

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- We denote the projected data as $\mathbf{x}'_n \in U$ and their coordinates by $\mathbf{z}_n$

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$$\mathbb{V}ar(z_1) = \frac{1}{N}\sum_{n=1}^{N} z_{1n}^2 = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{b}_1^T\mathbf{x}_n)^2 =$$

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where S is the sample covariance matrix.

Problem Setting of PCA

- We can describe the information contained in the data by looking at the spread of the data and measure it with **variance**
- In this setting, retaining most information after data compression is equivalent to capturing the largest amount of variance in the low-dimensional representation
- We maximize the variance of the low-dimensional code using a sequential approach.
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where S is the sample covariance matrix.

- Note that if we would not put a unit vector contraint on $\mathbf{b}_1$, the variance would increase for longer-length $\mathbf{b}_1$.

Mathematical Derivations

We need to solve the following constrained optimization problem

$$\max_{\mathbf{b}_1} \mathbf{b}_1^T S \mathbf{b}_1$$

$$\text{subject to } \|\mathbf{b}_1\|^2 = 1$$

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Finding the partial derivatives w.r.t. $\mathbf{b}_1$ and λ_1

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Setting these partial derivatives to 0 gives us

$$S\mathbf{b}_1 = \lambda_1 \mathbf{b}_1$$
$$\mathbf{b}_1^T \mathbf{b}_1 = 1$$

Does this look familiar?

Mathematical Derivations

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To obtain the projection of $\mathbf{x}_n$ on the obtained subspace, we can use the following formula

$$\mathbf{x}'_n = \mathbf{b}_1 z_{1n} = \mathbf{b}_1 \mathbf{b}_1^T \mathbf{x}_n \in \mathbb{R}^D$$

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$$\hat{\mathbf{X}} = \mathbf{X} - \sum_{i=1}^{m-1} \mathbf{b}_i \mathbf{b}_i^T \mathbf{X} = \mathbf{X} - \mathbf{B}_{m-1}\mathbf{X},$$

where $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_N] \in \mathbb{R}^{D \times N}$ and $\mathbf{B}_{m-1} = \sum_{i=1}^{m-1} \mathbf{b}_i \mathbf{b}_i^T$ is the projection matrix onto the subspace spanned by $\mathbf{b}_1, \ldots, \mathbf{b}_{m-1}$.

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- The m-th PC can be found by maximizing the variance

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$$\text{subject to } \|\mathbf{b}_m\|^2 = 1$$

where $\hat{S}$ is the covariance matrix of $\hat{\mathbf{X}}$

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  where $\hat{S}$ is the covariance matrix of $\hat{\mathbf{X}}$
- $\mathbf{b}_m$ is also an eigenvector of S and $\mathbb{V}ar(z_m) = \mathbf{b}_m^T S \mathbf{b}_m = \lambda_m$ is the m-th largest eigenvalue of S

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- We can reduce the dimensionality of our data, by using the M eigenvectors of the covariance matrix S associated with the M largest eigenvalues.

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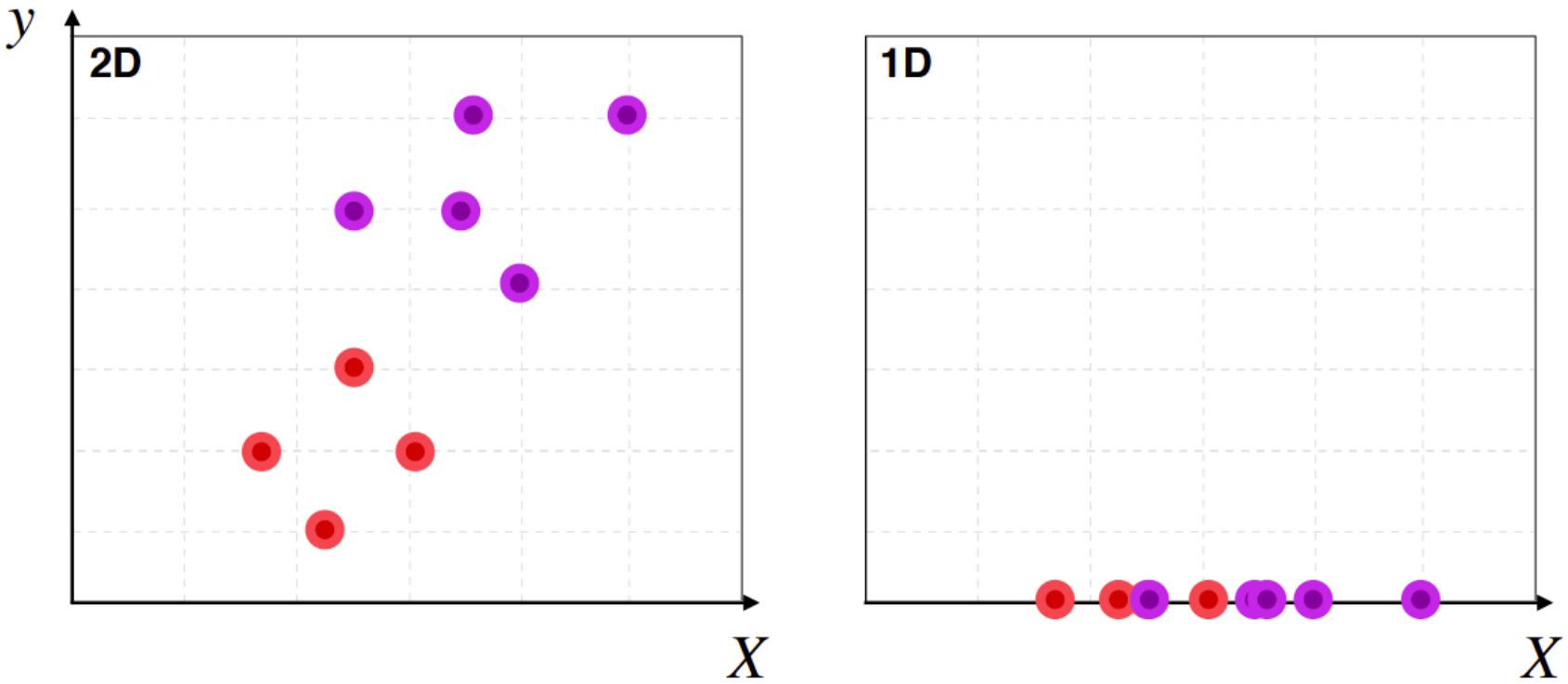
- The variance lost by data compression via PCA is

$$\sum_{i=M+1}^{D} \lambda_m$$

Intuition behind t-SNE



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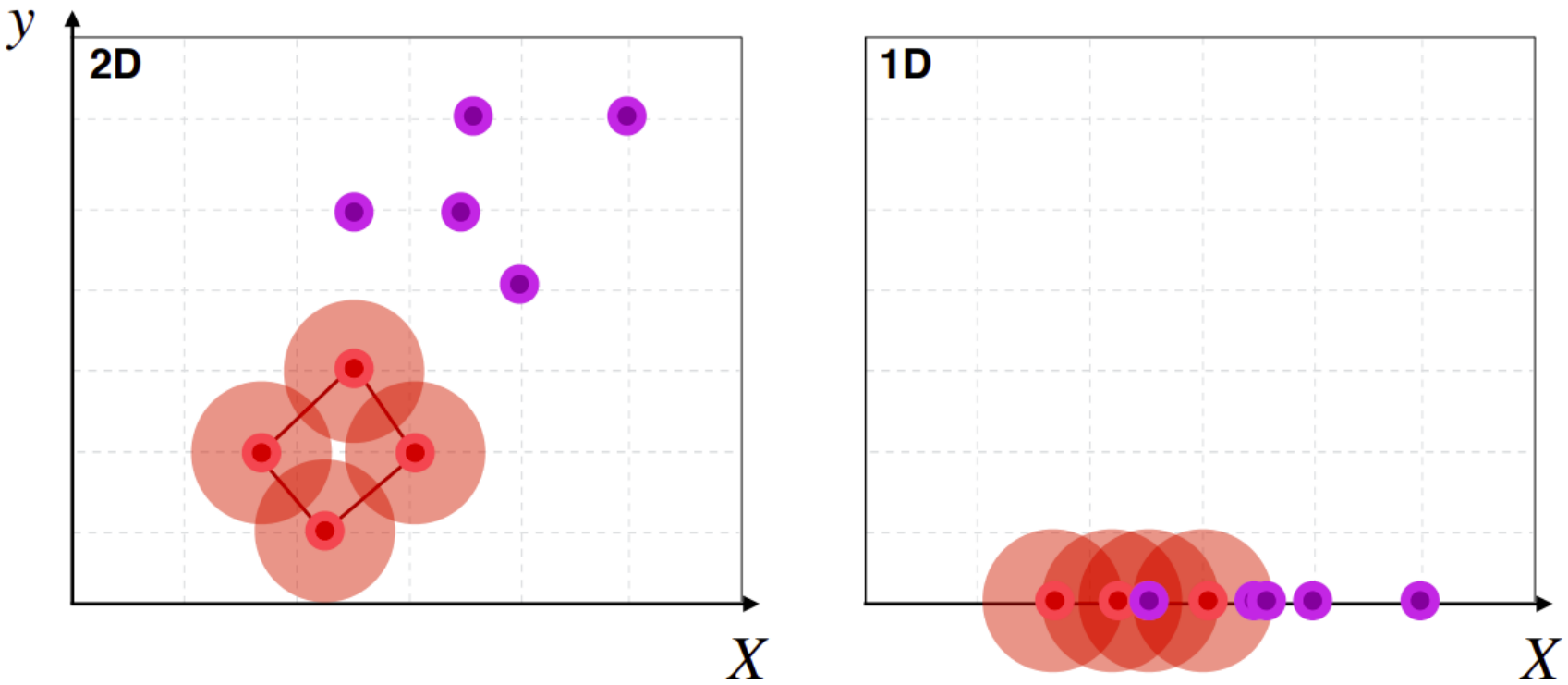

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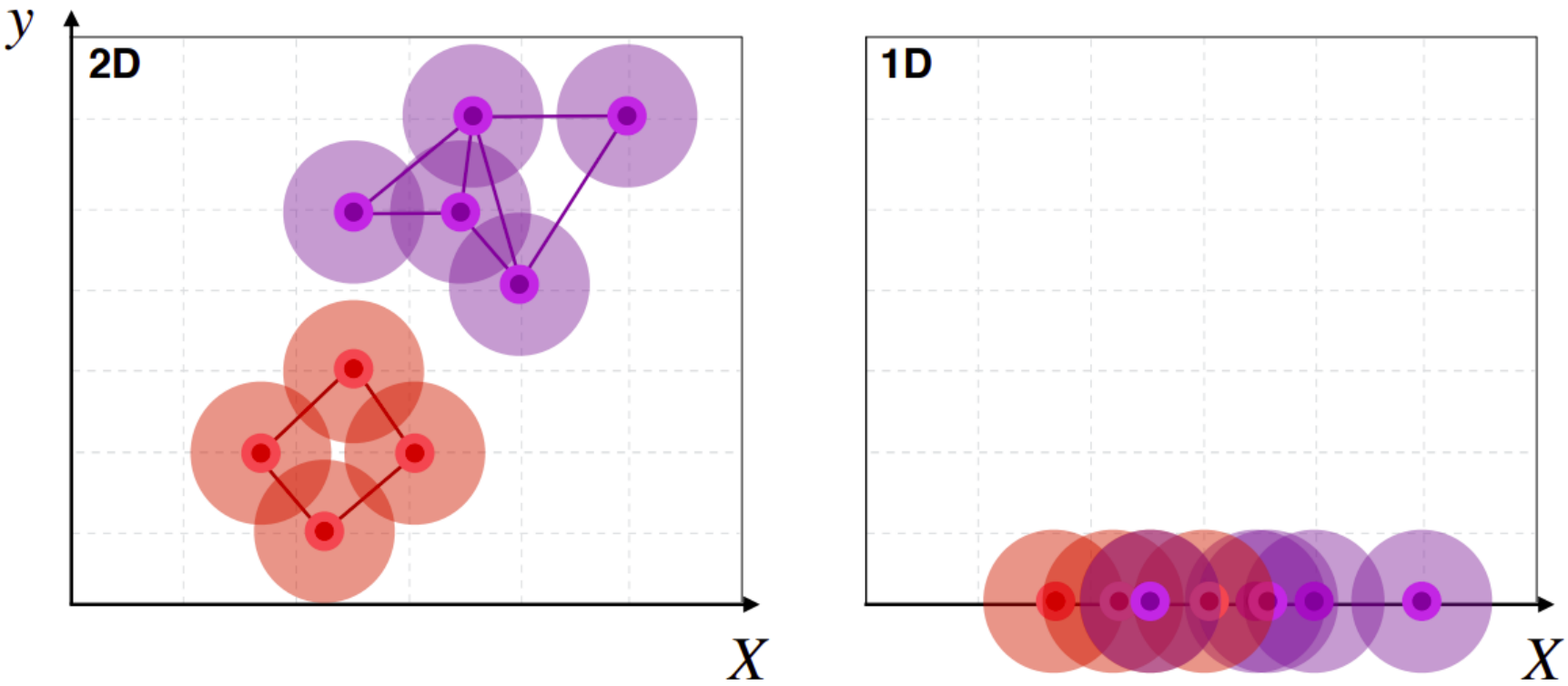

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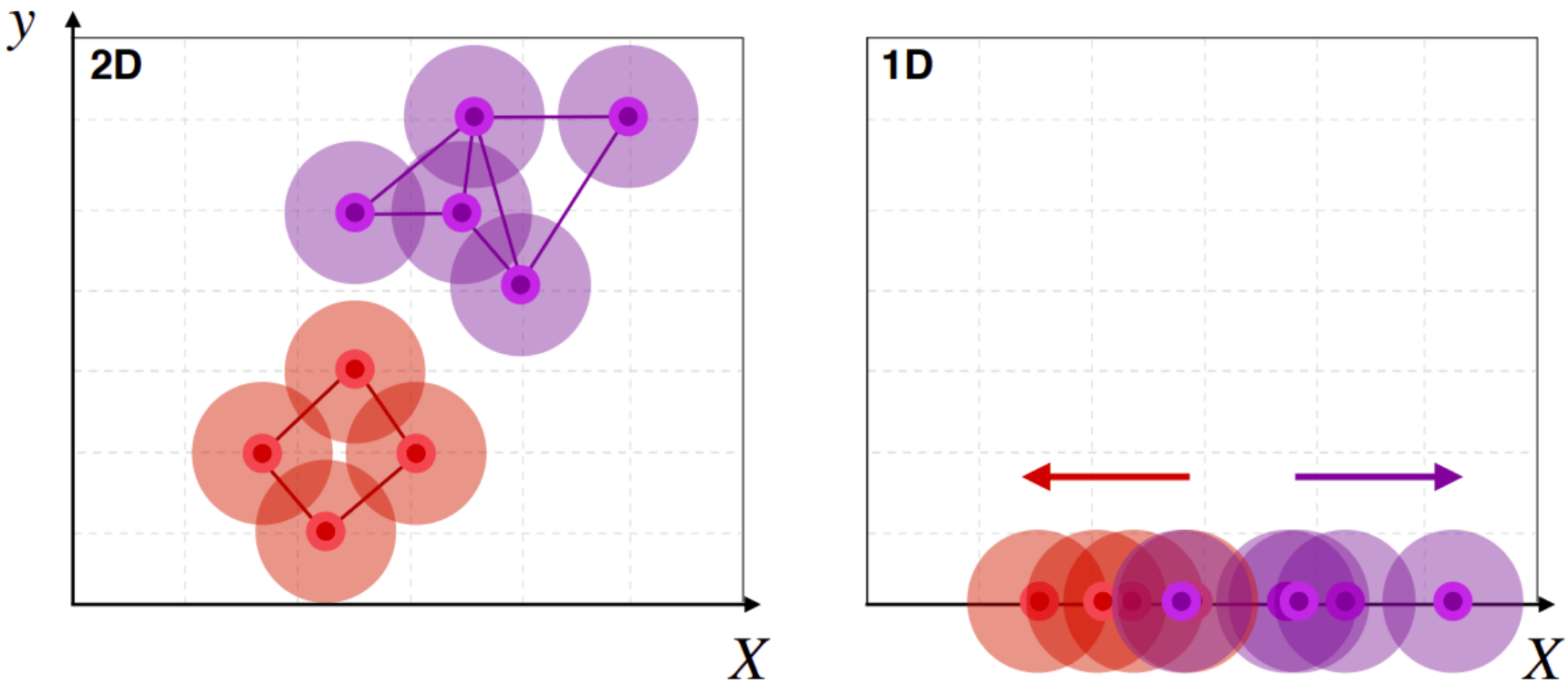

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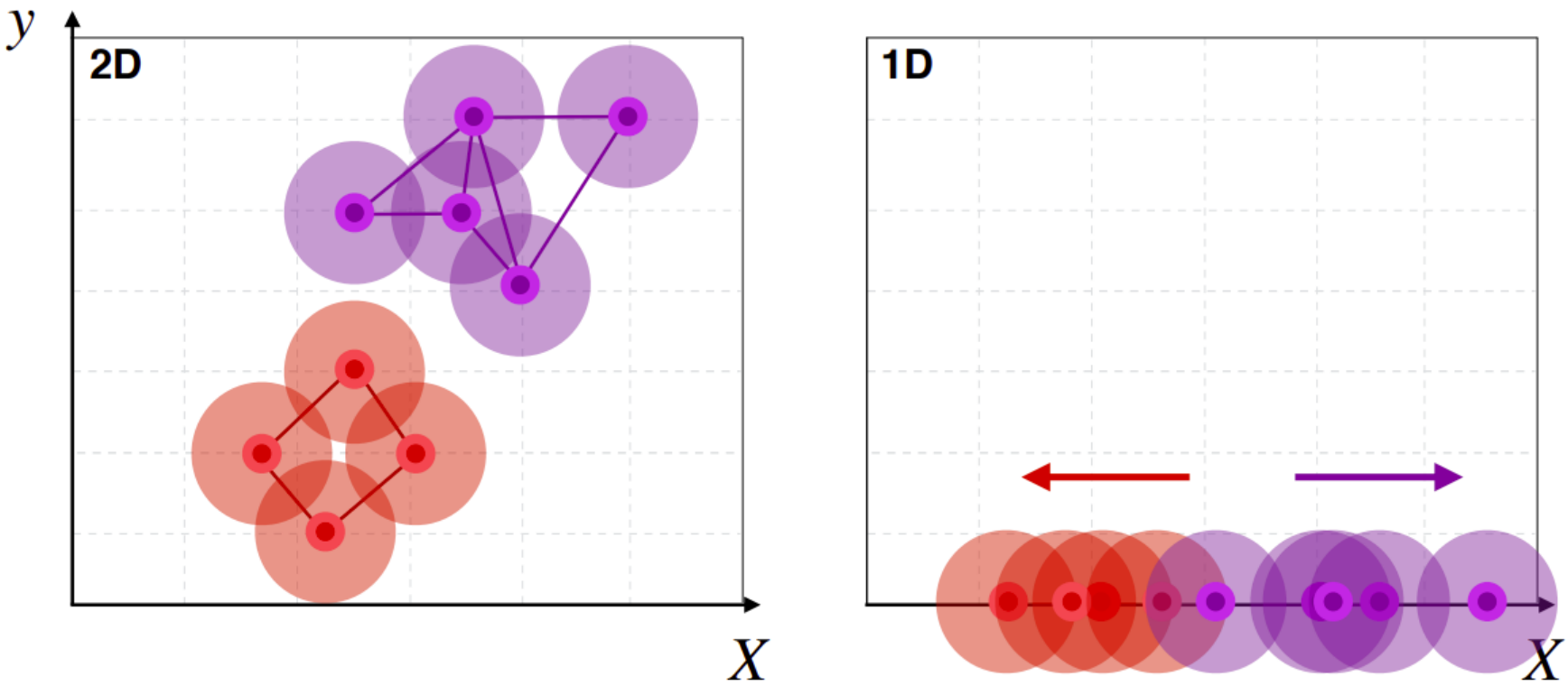

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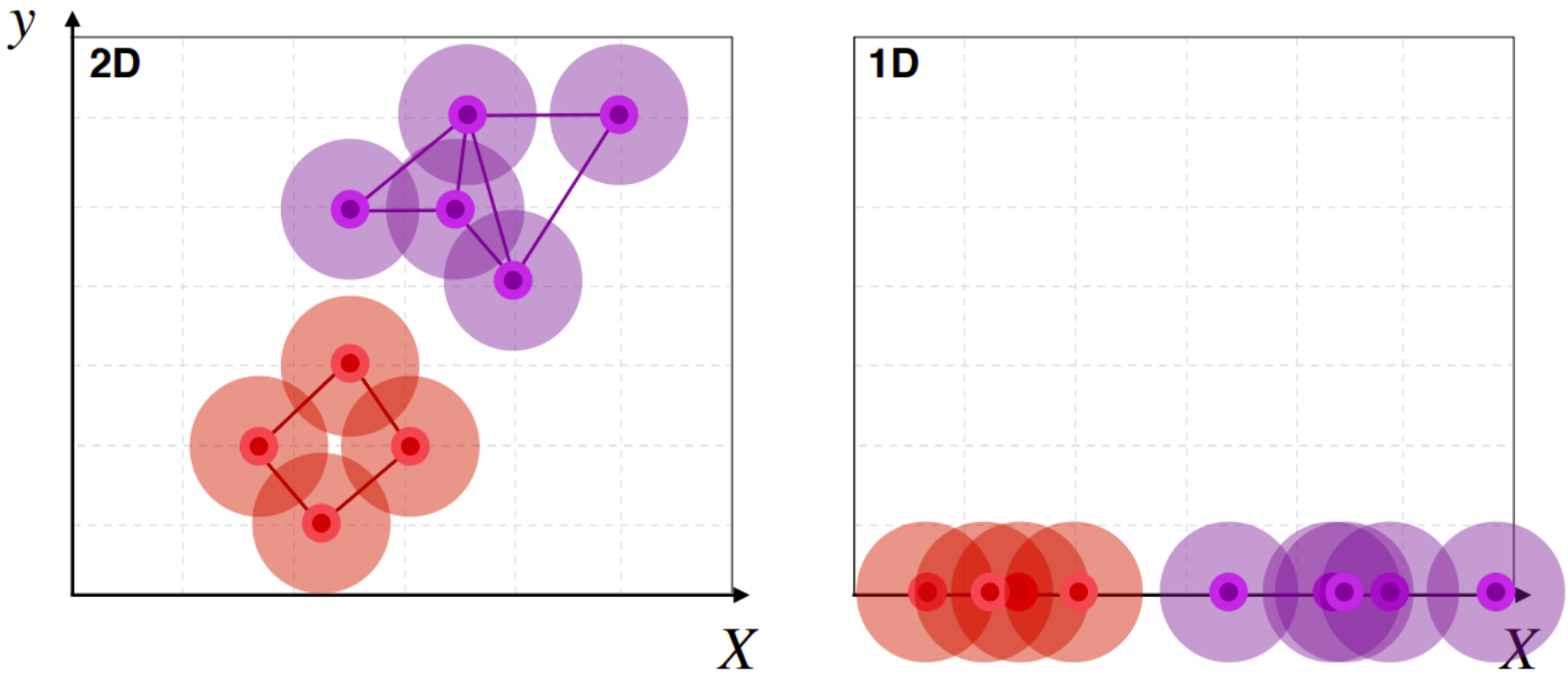
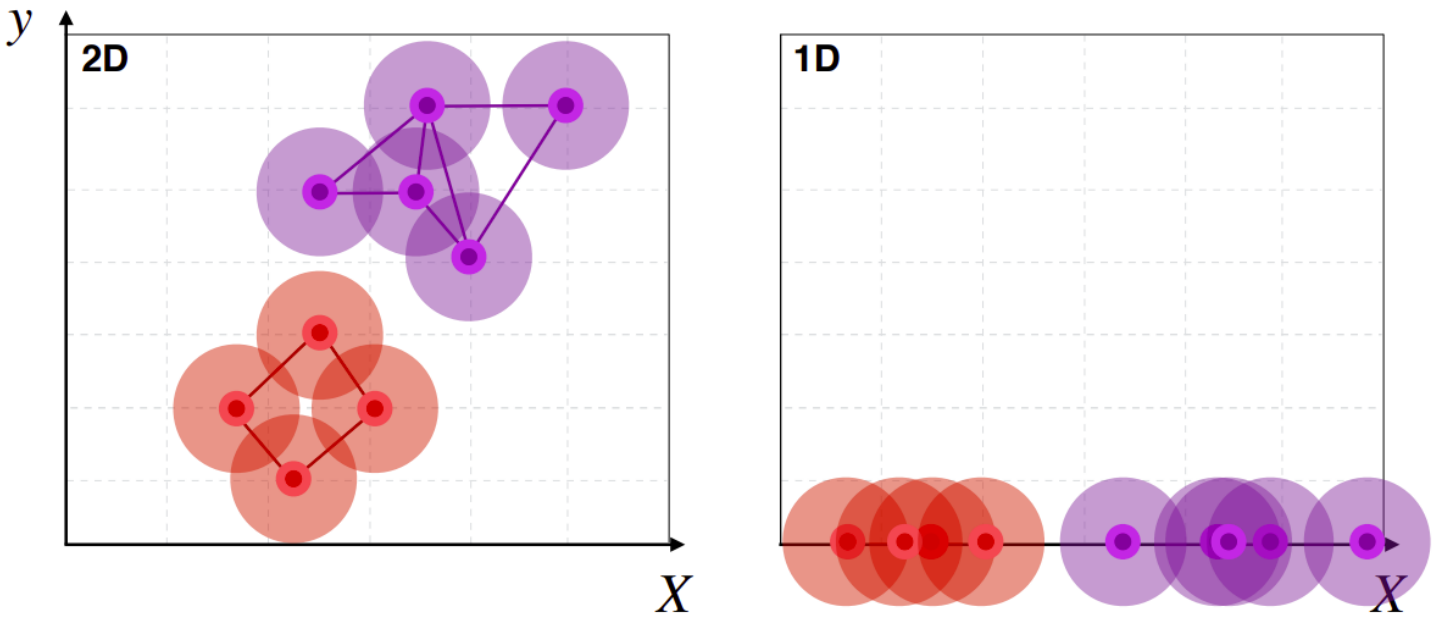


Intuition behind t-SNE

t-SNE iteratively tries to make distances in low-dimensional space to be similar to distances in high-dimensional space



What have we learned today?

- ✓ Dimensionality Reduction
- ✓ Principal Component Analysis
- ✓ t-Distributed Stochastic Neighbor Embedding (t-SNE)