JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN

UNDERSTANDING THE 6-DIM DATA

RESULTS FROM PRINCIPAL COMPONENTS ANALYSIS AND SELF-ORGANIZING MAPS

STEPHANIE KÄS

Belle II

Experimental Physics II

MINI-WORKSHOP
ANOMALY DETECTION WITH NEURAL NETWORKS
GIESSEN 21.02.2020

ATTENTION

This event will be photographed.

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OVERVIEW

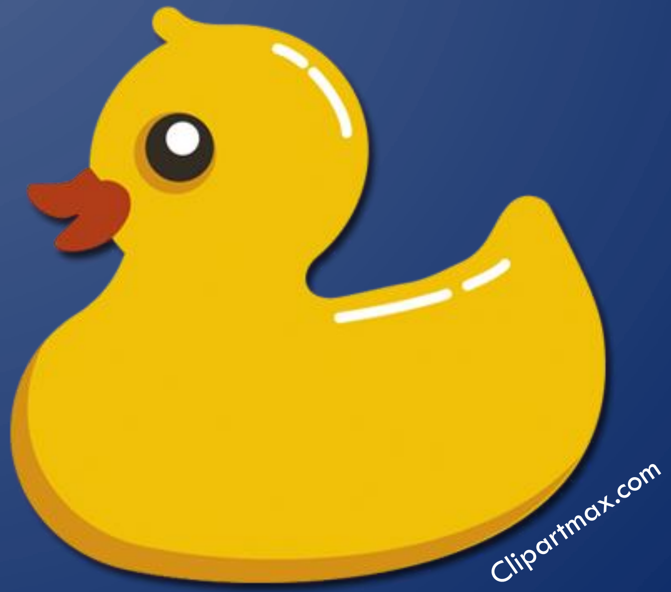
1. Principal components analysis
2. Antideuteron data set
3. Results of bachelor‘s thesis

PART 1

PRINCIPAL COMPONENTS ANALYSIS

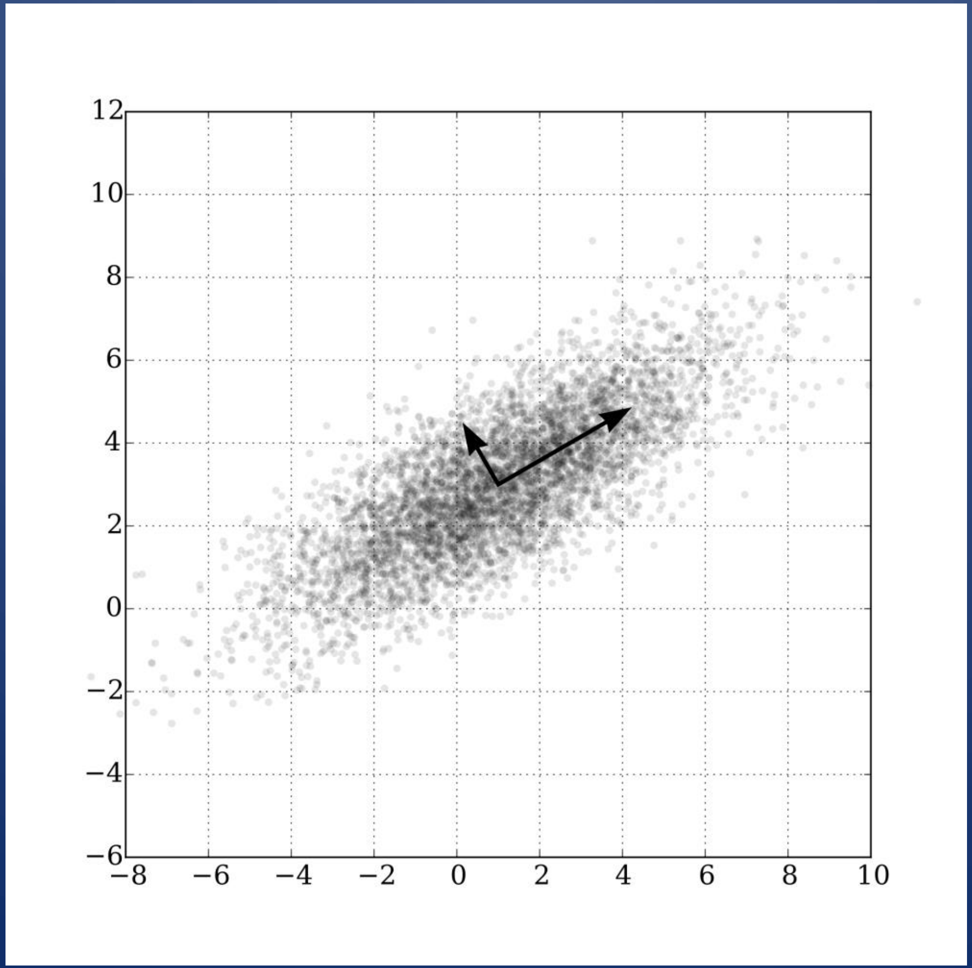
PRINCIPAL COMPONENTS ANALYSIS
IDEA

3D duck



2D duck

PRINCIPAL COMPONENTS ANALYSIS
DETAILS



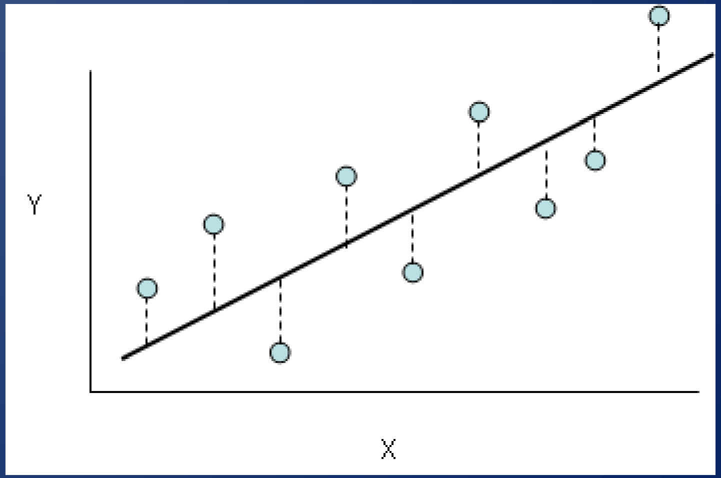
Wikipedia.org

PRINCIPAL COMPONENTS ANALYSIS
DETAILS

Given: data set of n attributes

Find n new axes by

- Minimization of error squares
- Maximization of variance



spcforexcel.com

PRINCIPAL COMPONENTS ANALYSIS
BASIC STATISTICS

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Covariance matrix

$$\Sigma = \begin{pmatrix} var(\vec{x}) & cov(\vec{x},\vec{y}) \\ cov(\vec{x},\vec{y}) & var(\vec{x}) \end{pmatrix}$$

For data set with two attributes $\vec{x}, \vec{y}$

Correlation matrix = normalized covariance matrix

PRINCIPAL COMPONENTS ANALYSIS
DETAILS

Find transformation matrix Γ so that Λ is diagonal.

$$\Lambda = \Gamma^T \Sigma \Gamma = \begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_n \end{pmatrix}$$

Columns of Γ are the axes of the new coordinate system.

PRINCIPAL COMPONENTS ANALYSIS
DETAILS

Higher values of λ_i $\leftrightarrow$ higher information content

$$\Lambda = \Gamma^T \Sigma \Gamma = \begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_n \end{pmatrix}$$

$$\lambda_1 \geq \lambda_2 \ldots \geq \lambda_n$$

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PROJECT 1

MULTIPARAMETER ANALYSIS OF ANTIDEUTERONS

Eigenvalues

λ_i	Cum. Sum [%]
2.73	45.46
2.03	79.28
0.62	89.62
0.47	97.55
0.12	99.54
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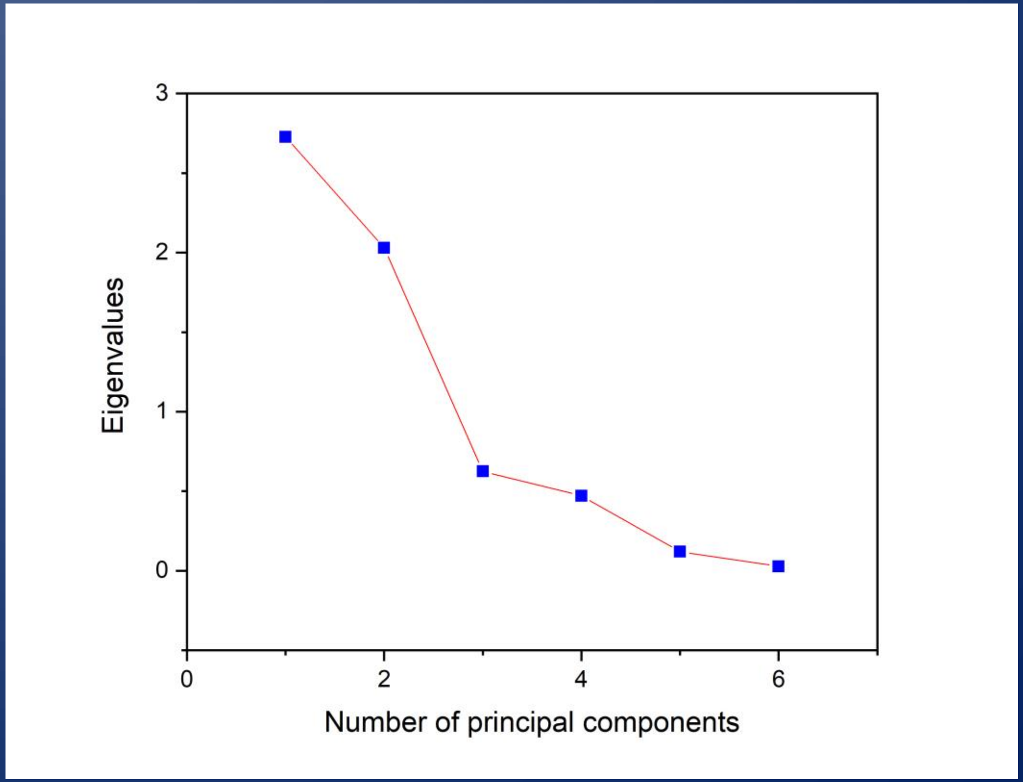
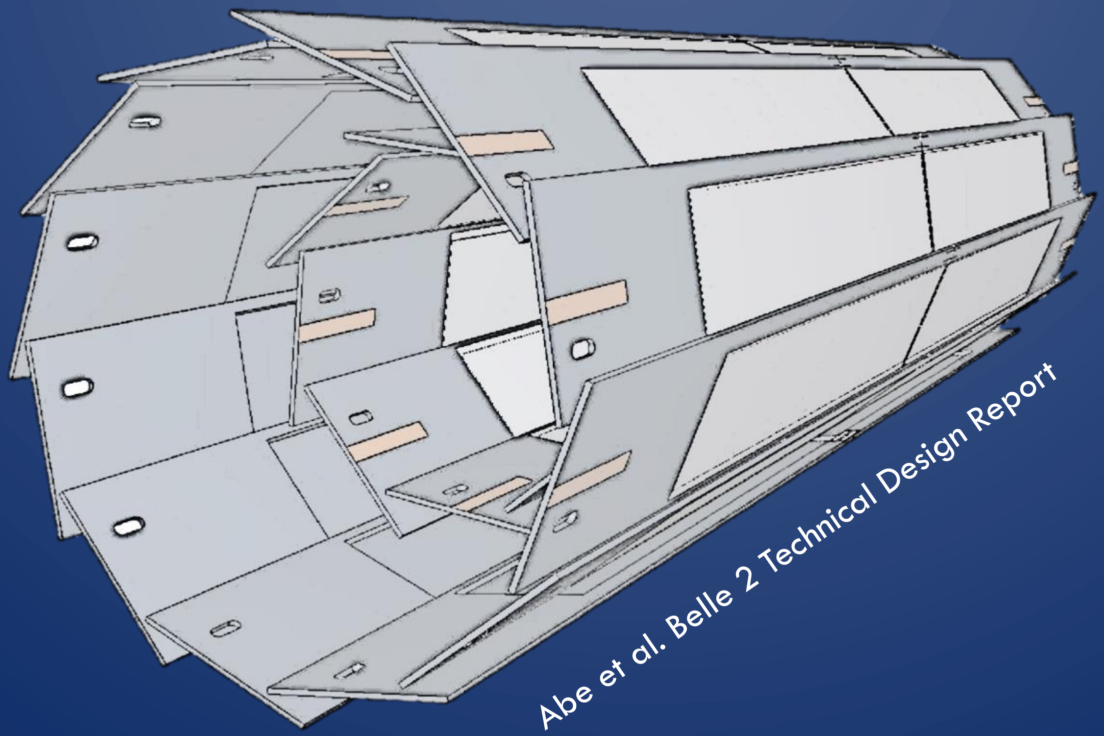
Scree graph (PXD)



PART 2

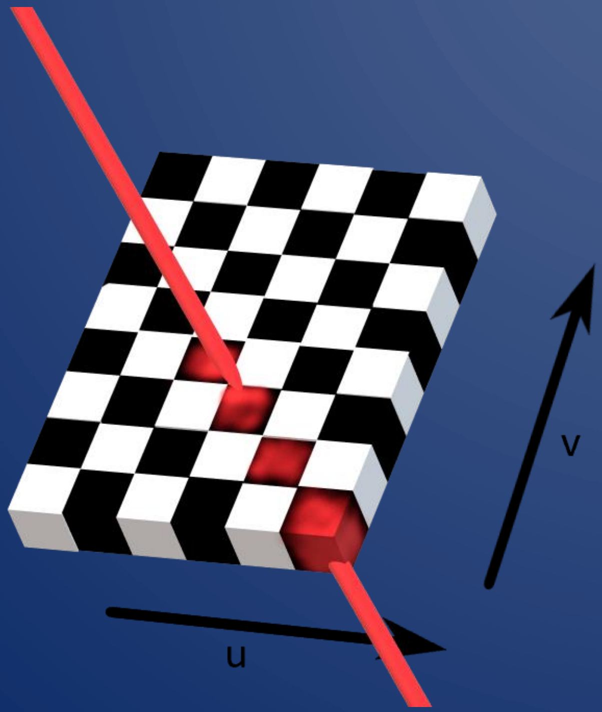
PIXEL DETECTOR'S ANTIDEUTERON DATA SET

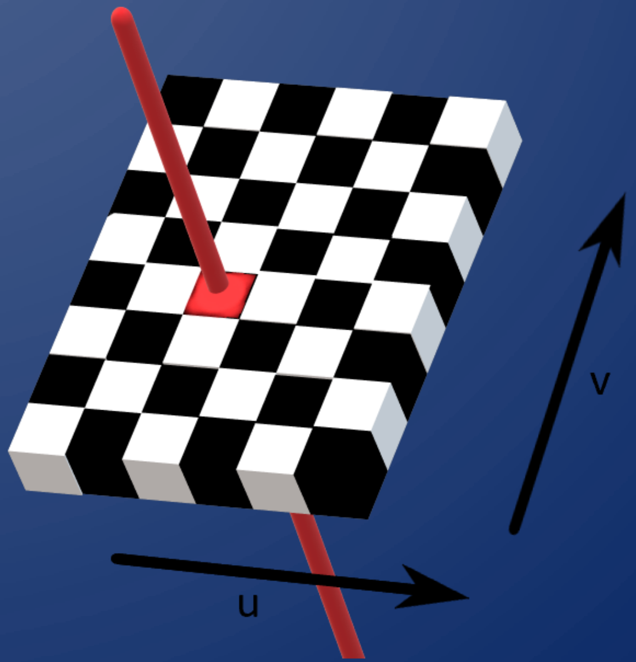
PIXEL DETECTOR



Abe et al. Belle 2 Technical Design Report

PIXEL DETECTOR



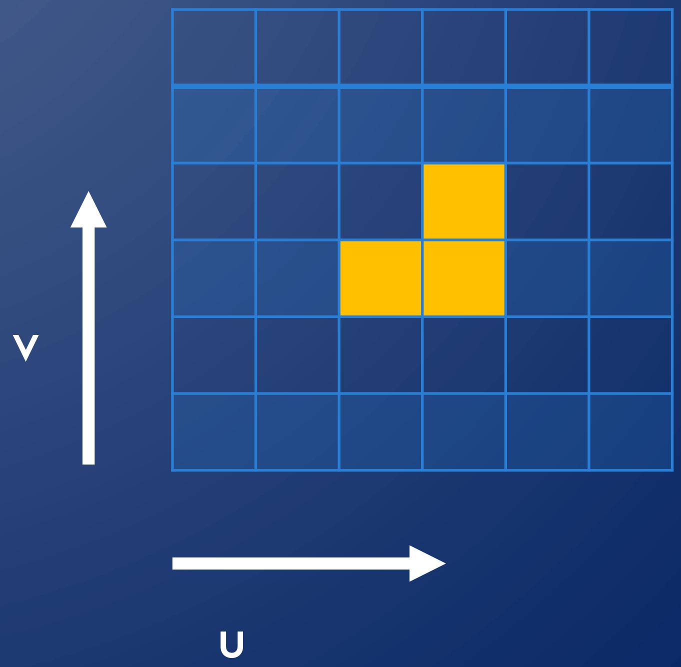


PIXEL DETECTOR
THE ANTIDEUTERON DATA SET

Group pixels into clusters

Cluster properties

- Total charge
- Seed charge
- Minimum charge



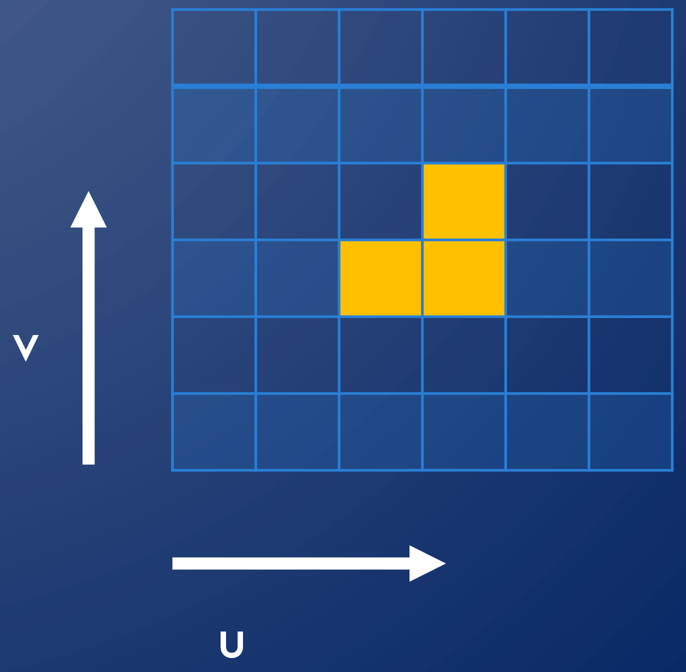
PIXEL DETECTOR
THE ANTIDEUTERON DATA SET

Group pixels to clusters

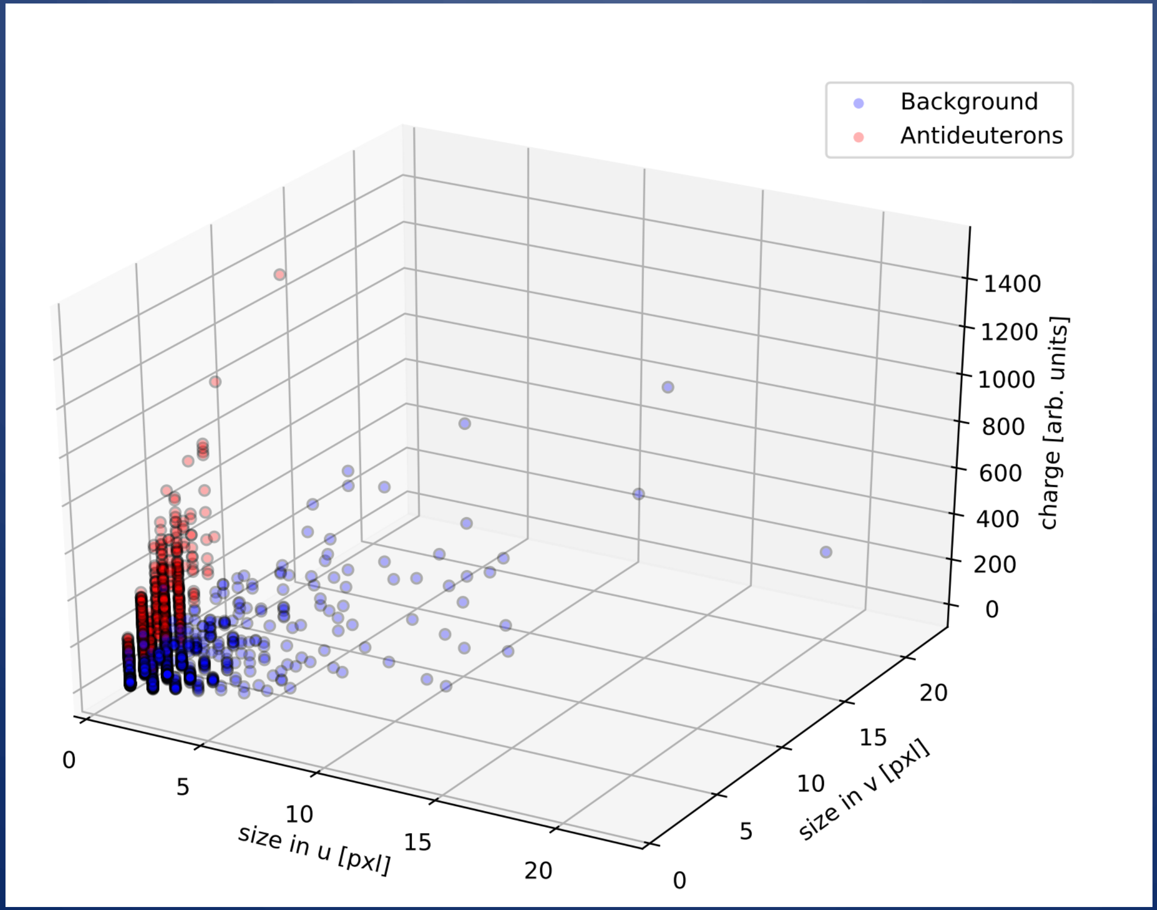
Cluster properties

- Total charge
- Seed charge
- Minimum charge

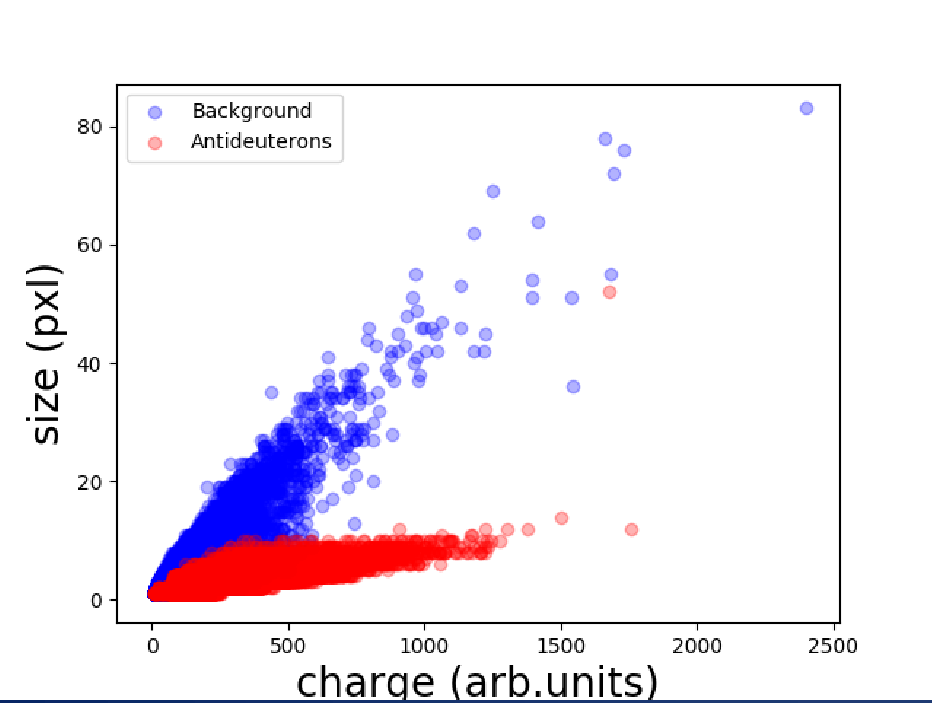
- Total size
- Size in u
- Size in v

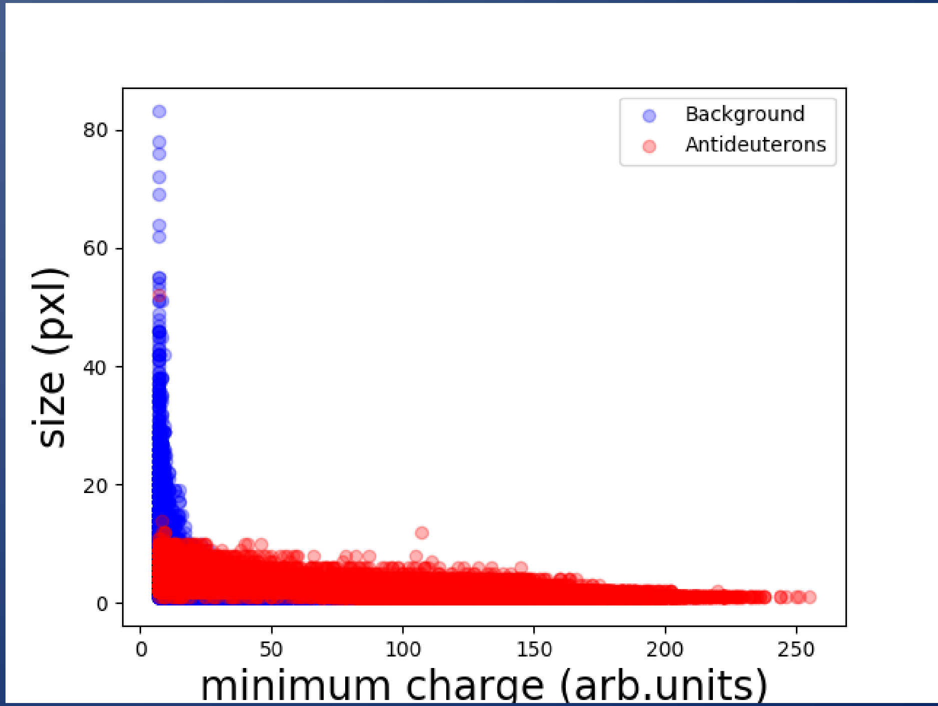


PIXEL DETECTOR
THE ANTIDEUTERON DATA SET



PIXEL DETECTOR
THE ANTIDEUTERON DATA SET





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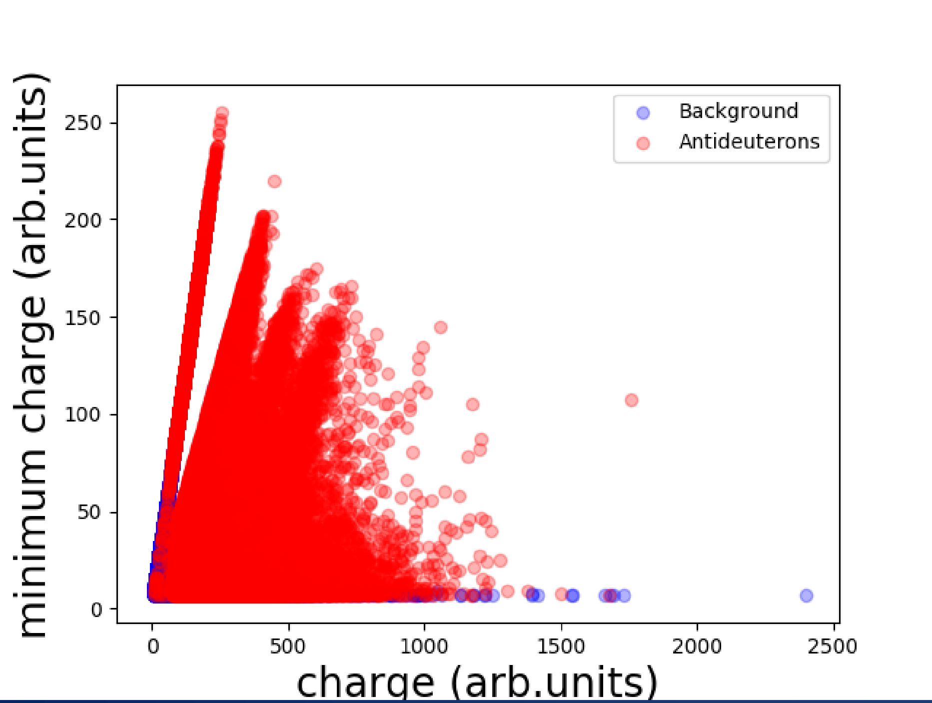
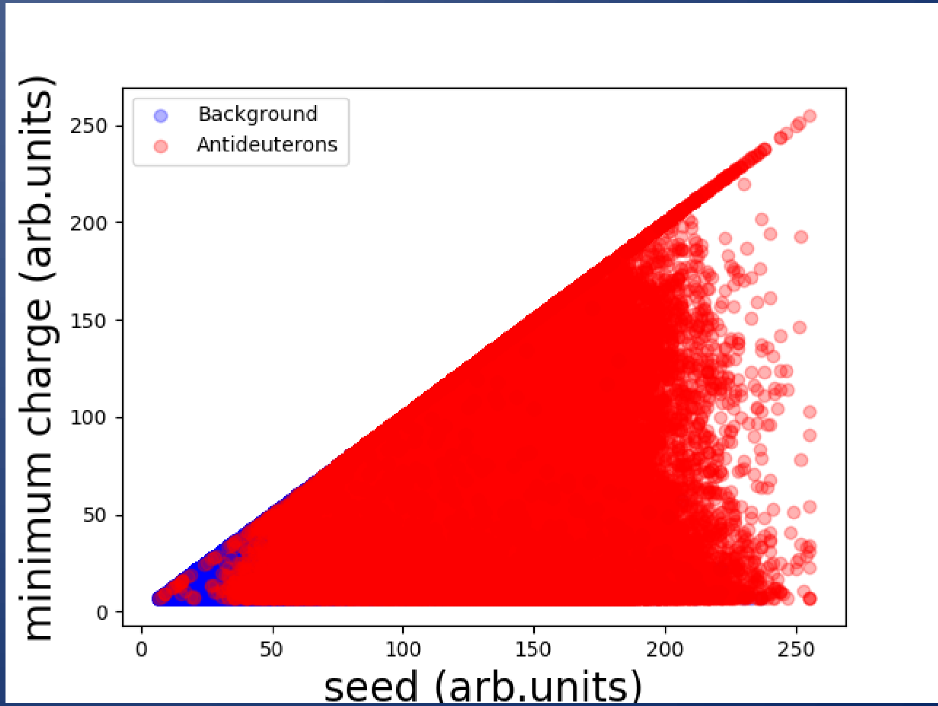
PIXEL DETECTOR
THE ANTIDEUTERON DATA SET





PART 3

BACHELOR'S THESIS

BACHELOR‘S THESIS - GOALS

1. Goal: Better understanding of data set
   - Find correlations in cluster properties -> PCA
   - Cluster shapes
2. Goal: Separate particles from background
   - Use SOMs: Separate more than 2 particles from background
   - Is pre-transformation into PCA-space helpful?

PROJECT 1: MULTIPARAMETER ANALYSIS OF ANTIDEUTERONS

Which correlations between the 6 cluster properties exist ?

Try PCA!

PROJECT 1

MULTIPARAMETER ANALYSIS OF ANTIDEUTERONS

Correlation matrix (lower half)

Cluster Property	Charge	Min. Charge	Seed	Size	Size in u	Size in v
Charge	1					
Min. Charge	0.2233	1				
Seed	0.7854	0.4771	1			
Size	0.4617	-0.2882	0.0392	1		
Size in u	0.1596	-0.2600	-0.1399	0.8044	1	
Size in v	0.4144	-0.2091	0.0546	0.8414	0.4627	1

Several high correlations!

PROJECT 1

MULTIPARAMETER ANALYSIS OF ANTIDEUTERONS

Interpretation of principal components

PC1 = Measure for size

PC2 = Measure for charge

PC3 = ?

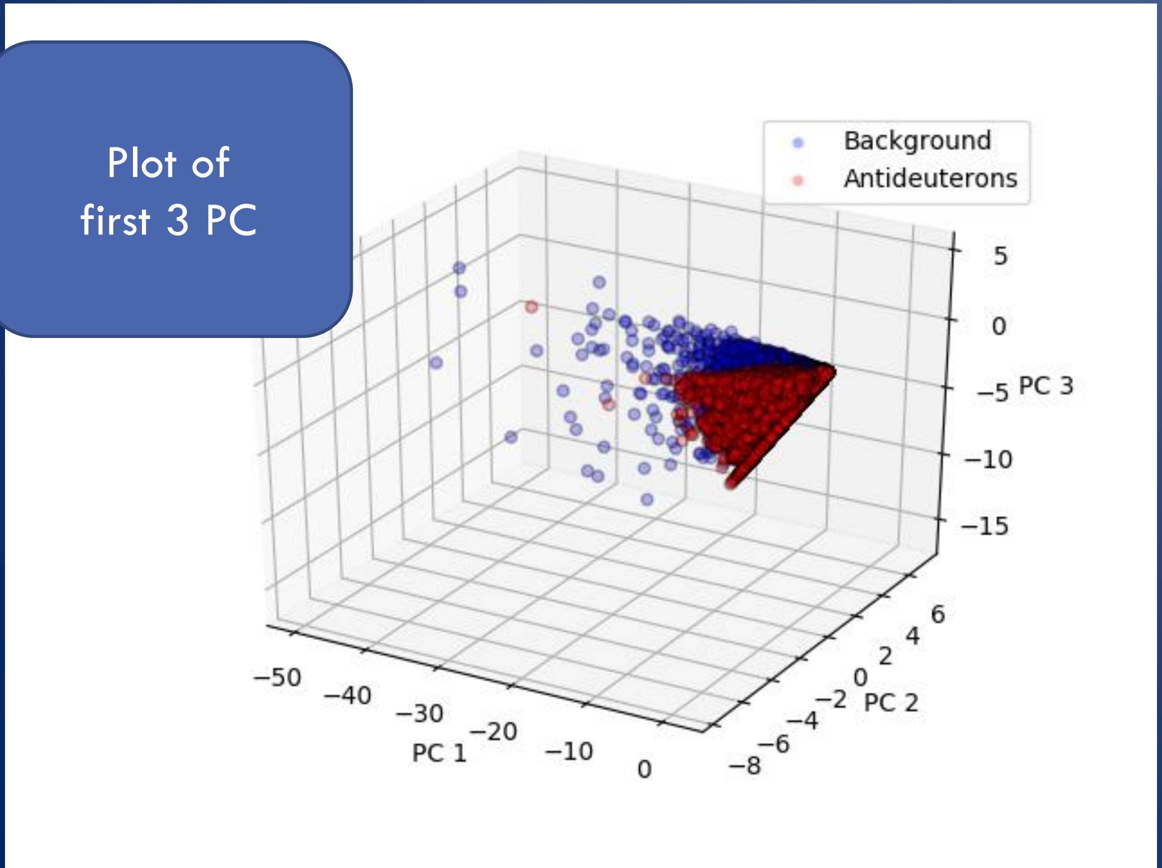
79.28 % of total information

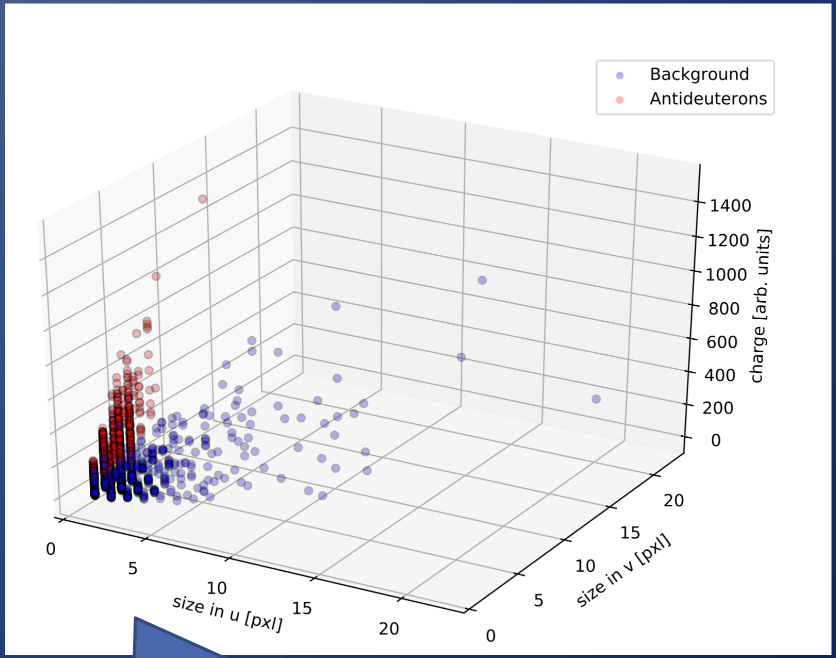
89.69 %

PROJECT 1

MULTIPARAMETER ANALYSIS OF ANTIDEUTERONS

Plot of first 3 PC



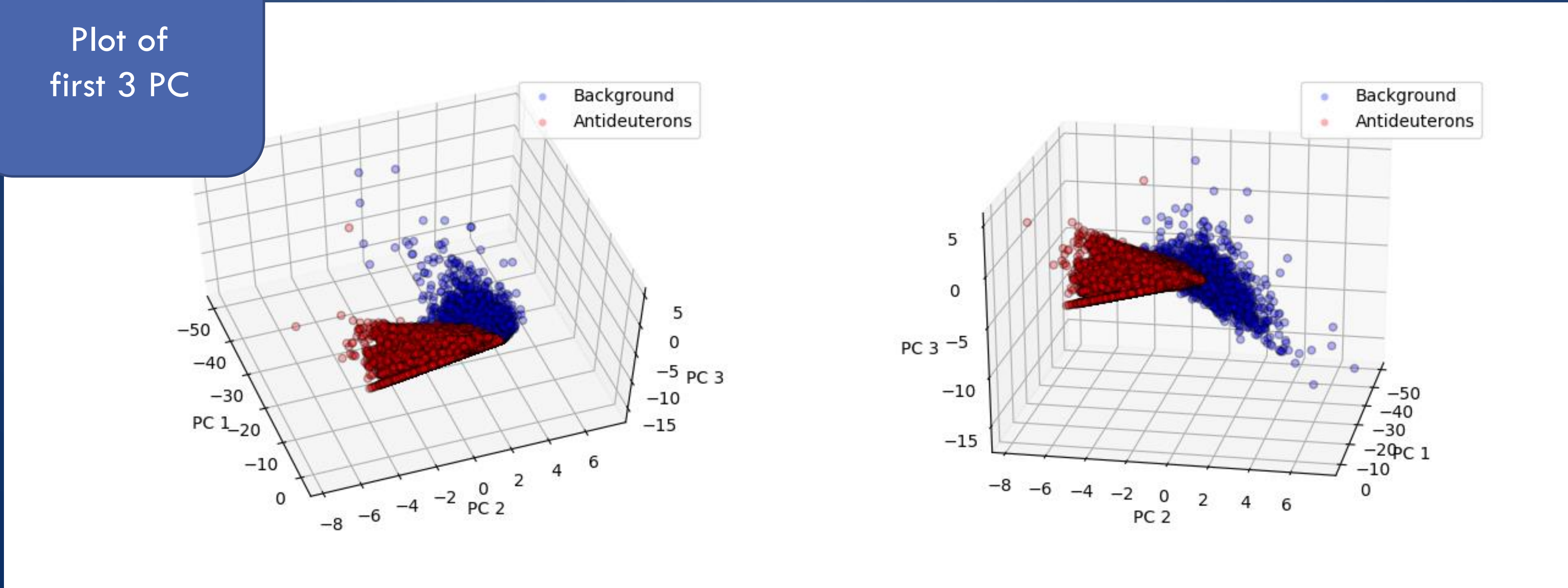


Original data set

PROJECT 1

MULTIPARAMETER ANALYSIS OF ANTIDEUTERONS

Plot of first 3 PC



BACHELOR‘S THESIS - RESULTS

Dimension can be reduced to 3D

PROJECT 2: DATA SEPARATION USING SOMS

Use reduced data set as input for SOMs.

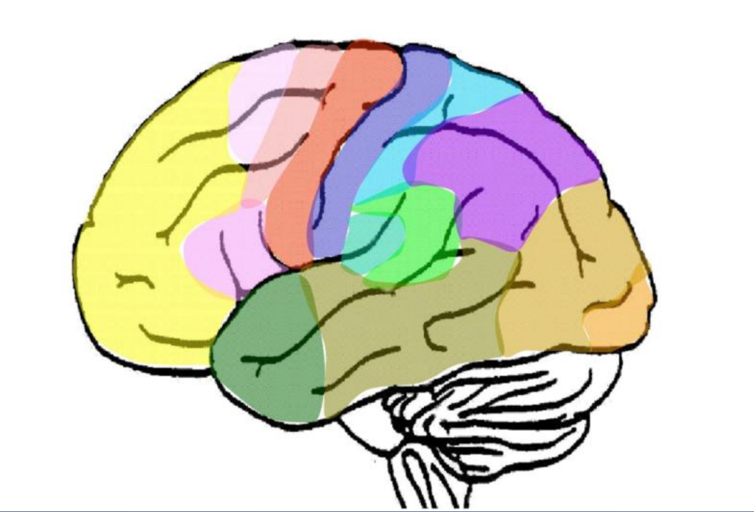
Try PCA & SOMs!

Does PCA-pre-transformation enhance SOM performance?

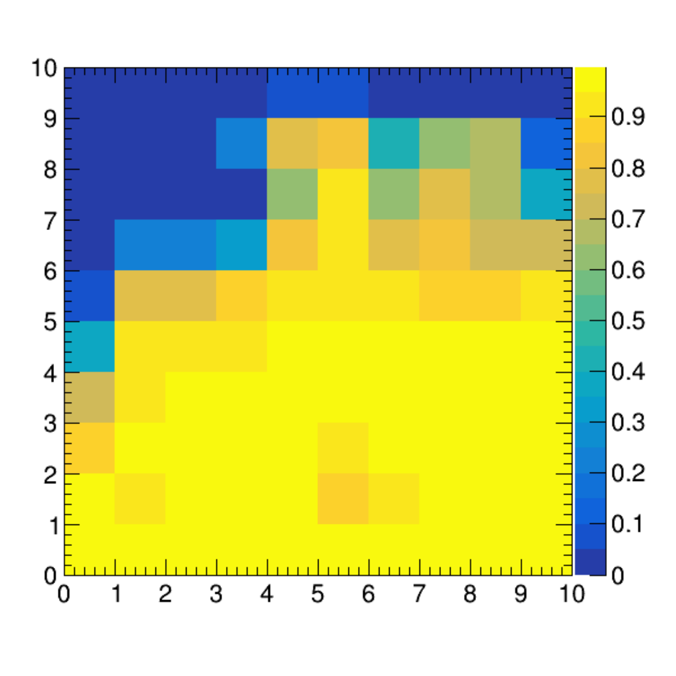
PROJECT 2: DATA SEPARATION USING SOMS

Idea: Separating particle signals from beam background

Method: Self-organizing maps



R. Westermann,
VL Neuroanatomie*



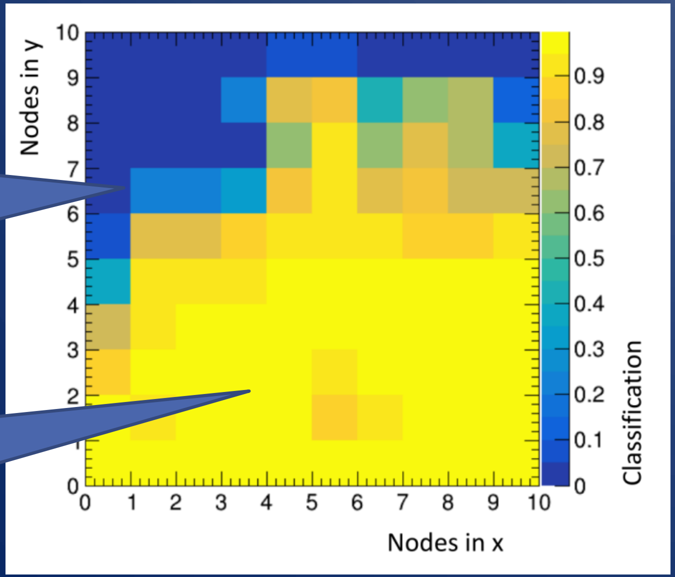
*Philipps Universität Marburg, SoSe 2016

PROJECT 2

DATA SEPARATION USING SOMS

ANTIDEUTERONS

ORIGINAL 6-DIM DATA SET



Background-like nodes

Antideuteron-like nodes

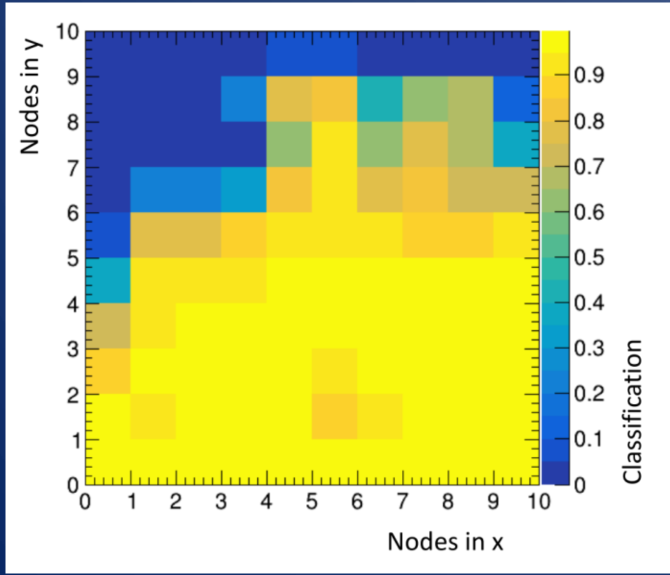
- Separation successful
- Results of Katharina's thesis confirmed

PROJECT 2

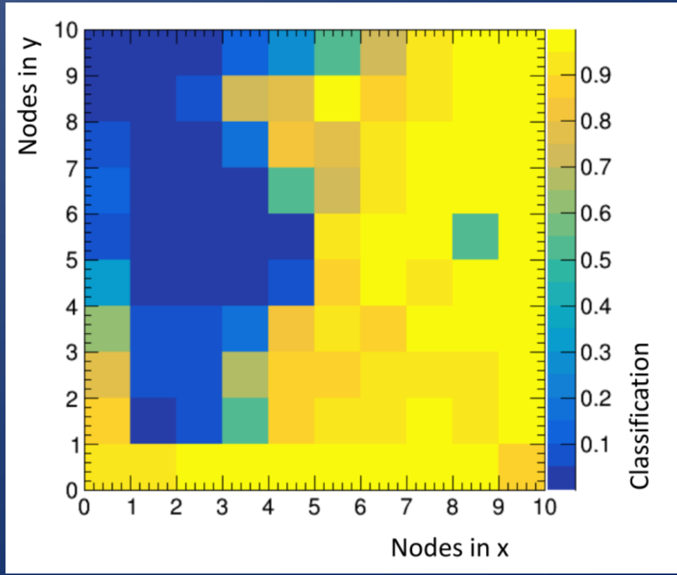
DATA SEPARATION USING SOMS

ANTIDEUTERONS

ORIGINAL 6-DIM DATA SET



PCA 6-DIM DATA SET



BACHELOR‘S THESIS - RESULTS

Dimension can be reduced to 3D

PCA does not enhance performance of SOMs

PROJECT 2

DATA SEPARATION USING SOMS

ANTIDEUTERONS, TETRAQUARKS AND PIONS

Can we separate 3 particles from background?

SOMs

Antideuterons, Tetraquarks and Pions

PROJECT 2

DATA SEPARATION USING SOMS

ANTIDEUTERONS, TETRAQUARKS AND PIONS

ROC-CURVES

"RECEIVER OPERATING CHARACTERISTIC"

Signal efficiency: True positive rate

$$P(classified\ as\ signal \mid signal)$$

Background rejection:

1- $P(classified\ as\ background \mid background)$

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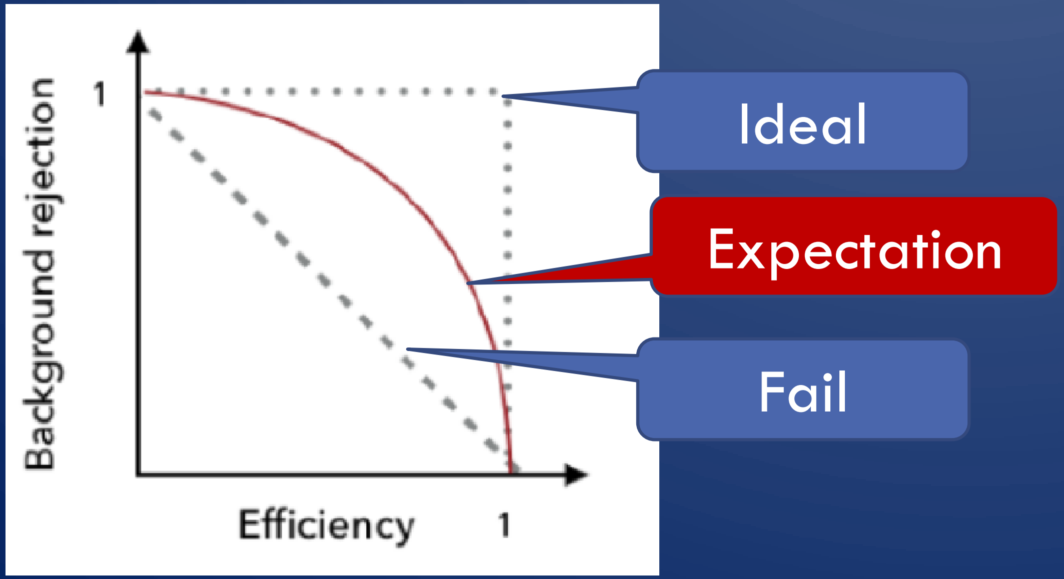
PROJECT 2

DATA SEPARATION USING SOMS

ANTIDEUTERONS, TETRAQUARKS AND PIONS

ROC-CURVES

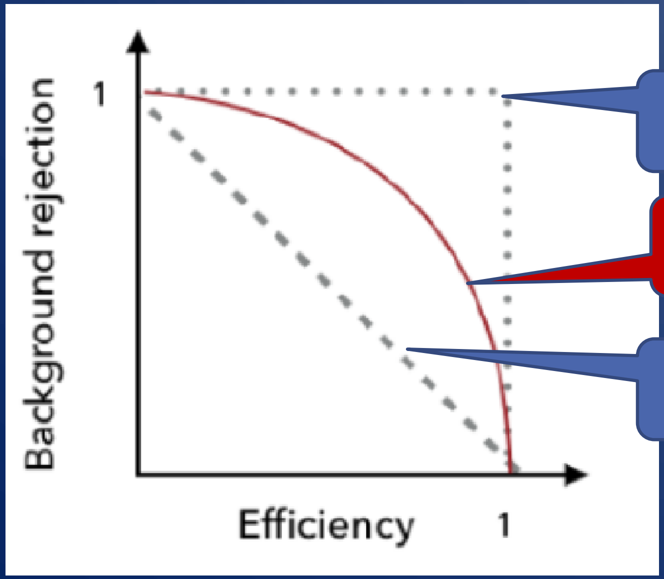


PROJECT 2

DATA SEPARATION USING SOMS

ANTIDEUTERONS, TETRAQUARKS AND PIONS

ROC-CURVES

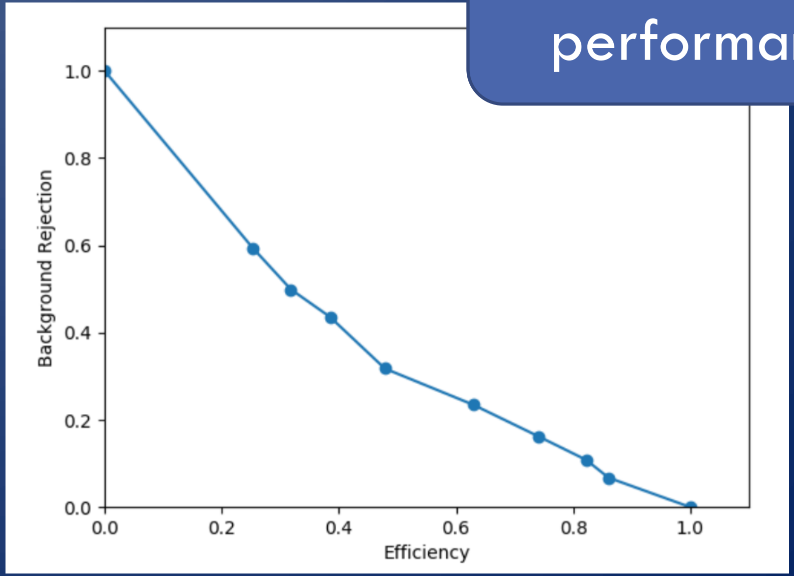


Ideal

Expectation

Fail

RESULT



Super bad performance!

BACHELOR'S THESIS - RESULTS

Dimension can be reduced to 3D

PCA does not enhance performance of SOMs

SOMs cannot separate more than 2 data types

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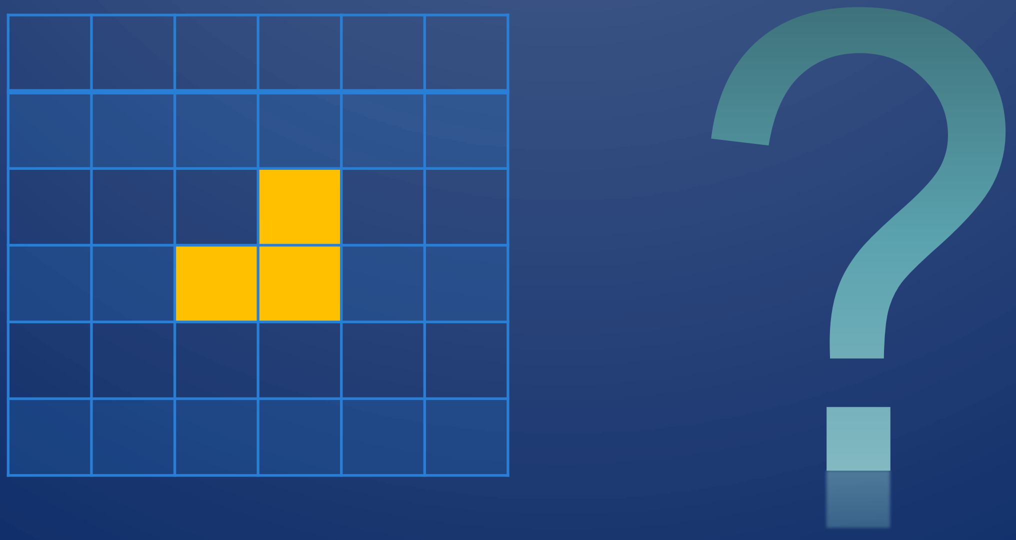
PROJECT 3: CLUSTER SHAPE ANALYSIS

Which cluster shapes do appear?



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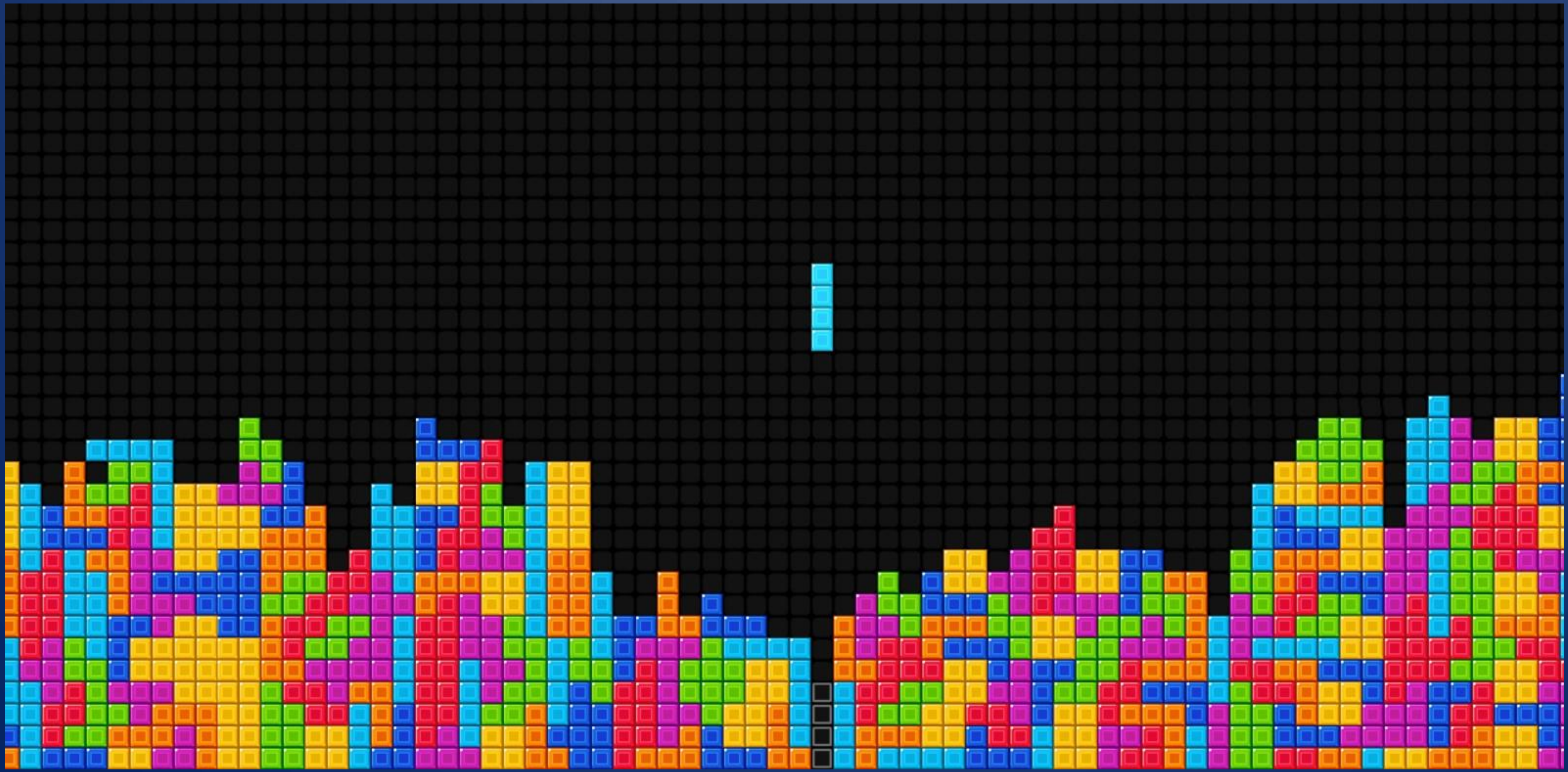
PROJECT 3

CLUSTER SHAPE ANALYSIS



wallpaperaccess.com/retro-game

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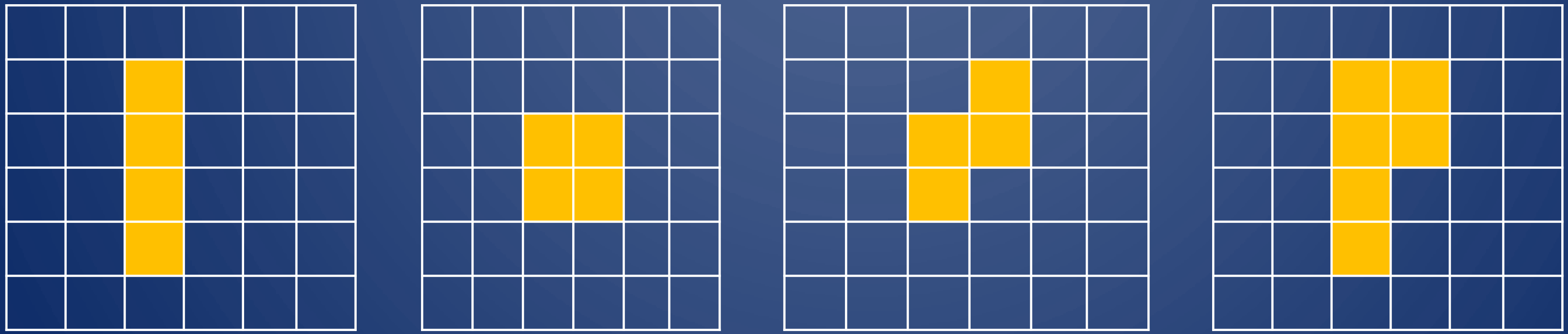
PROJECT 3

CLUSTER SHAPE ANALYSIS



Ca. 40% narrow rectangular

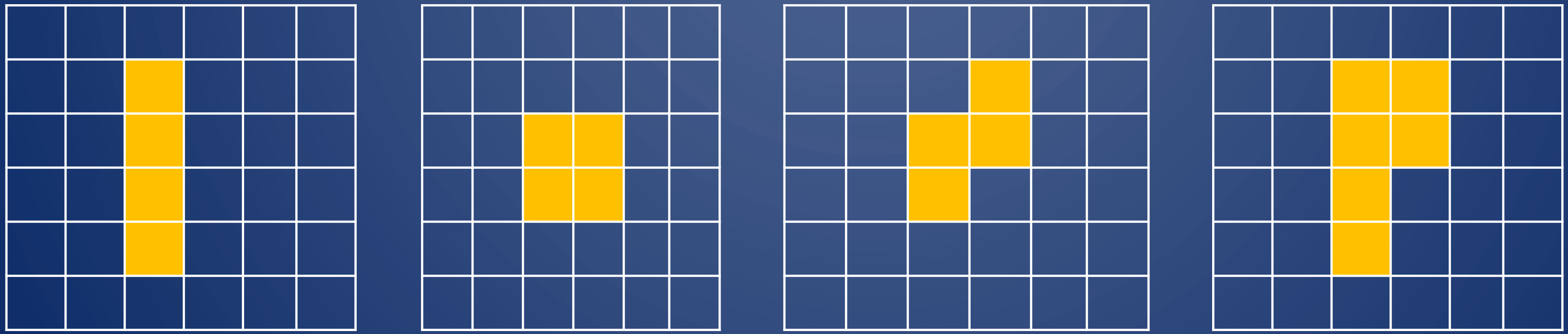
Ca. 17% squares

Ca. 1/3 2 pxl
Ca. 1/7 1 pxl

Ca. 10% > 6 pxl

PROJECT 3

CLUSTER SHAPE ANALYSIS



Pattern recognition?

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BACHELOR‘S THESIS - RESULTS

Dimension can be reduced to 3D

PCA does not enhance performance of SOMs

SOMs cannot separate more than 2 data types

PXD clusters come in many different shapes

POSSIBLE FUTURE PROJECTS

- Compare different versions of PCA and SOMs
- Use pattern recognition on cluster shapes
  - Try reinforcement learning?
- Try support vector machines

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Thank you

for your attention!

N-te

Background: quantumfbi.com

PART 4

DETAILS ON PCA

PRINCIPAL COMPONENTS ANALYSIS

BASIC STATISTICS

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Variance

$$var(\vec{x}) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{x})^2$$

measure of spread of x_i

PRINCIPAL COMPONENTS ANALYSIS

BASIC STATISTICS

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Variance

$$var(\vec{x}) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{x})^2$$

Empirical covariance

$$cov(\vec{x}, \vec{y}) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{x})(y_i - \hat{y})$$

indication for correlations between $\vec{x}$ and $\vec{y}$

PRINCIPAL COMPONENTS ANALYSIS

DETAILS

Higher values of λ_i $\leftrightarrow$ higher information content

$$\lambda_1 \geq \lambda_2 \dots \geq \lambda_n$$

Information percentage of axis i (cumulative sum):

$$\frac{\lambda_i}{\sum_{i=1}^{n} \lambda_i} \cdot 100\%$$

PRINCIPAL COMPONENTS ANALYSIS

CHOOSING NUMBER OF AXES

Critierion 1:

Choose only $\lambda_i \geq 1$

Criterion 2:

$$\frac{\lambda_i}{\sum_{i=1}^{n} \lambda_i} \cdot 100\% \geq 90\%$$

Criterion 3:

Cut at first rapid change of slope in *Scree graph*.

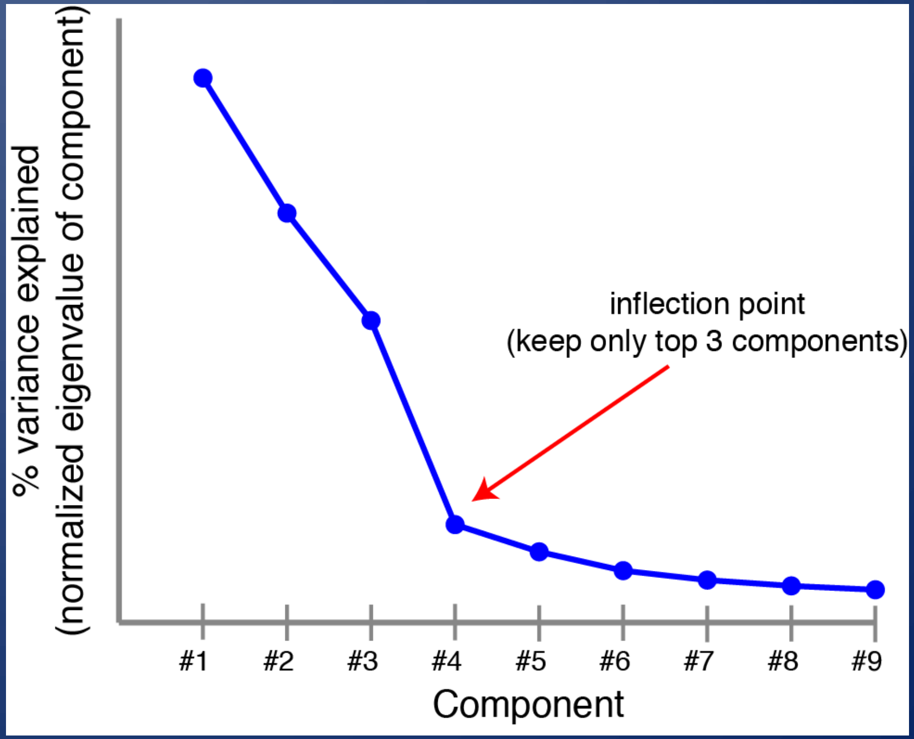
PRINCIPAL COMPONENTS ANALYSIS

CHOOSING NUMBER OF AXES

Criterion 3:

Cut at first rapid change of slope in *Scree graph.*

Scree graph (example)



alexhwilliams.info

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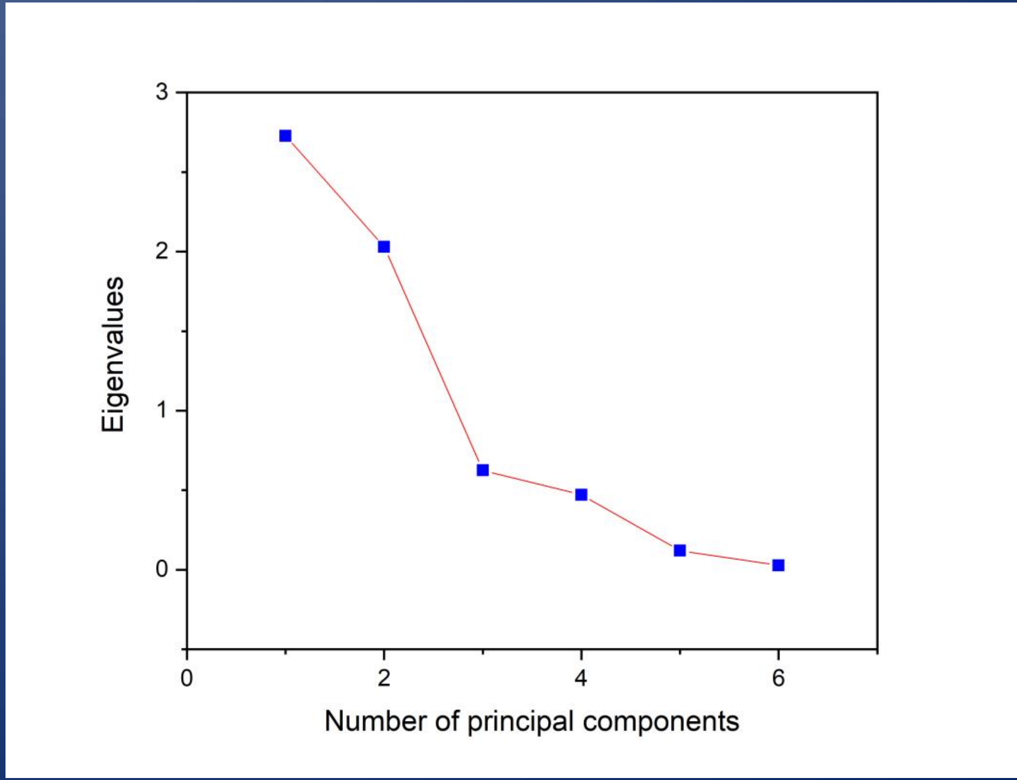

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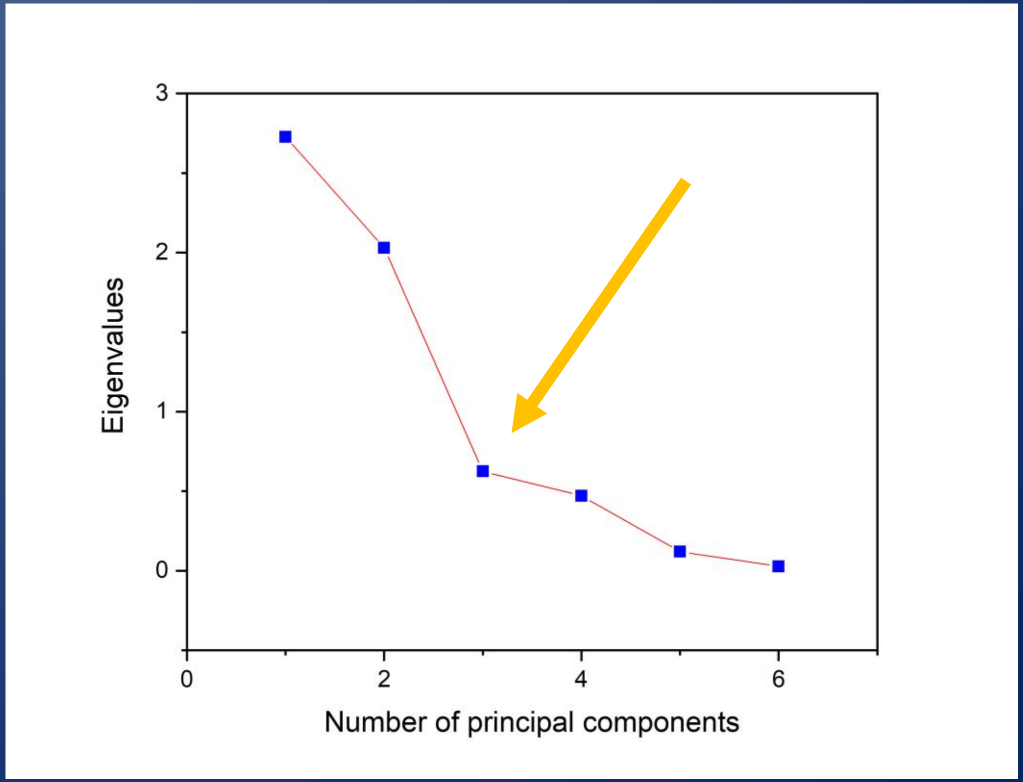
Scree graph



PRINCIPAL COMPONENTS ANALYSIS
IMPORTANT REMARKS

Pre-processing is a must:

- Normalisation is required
- PCA presumes linear correlations
- if non-linear:
  use *log* or *actan*

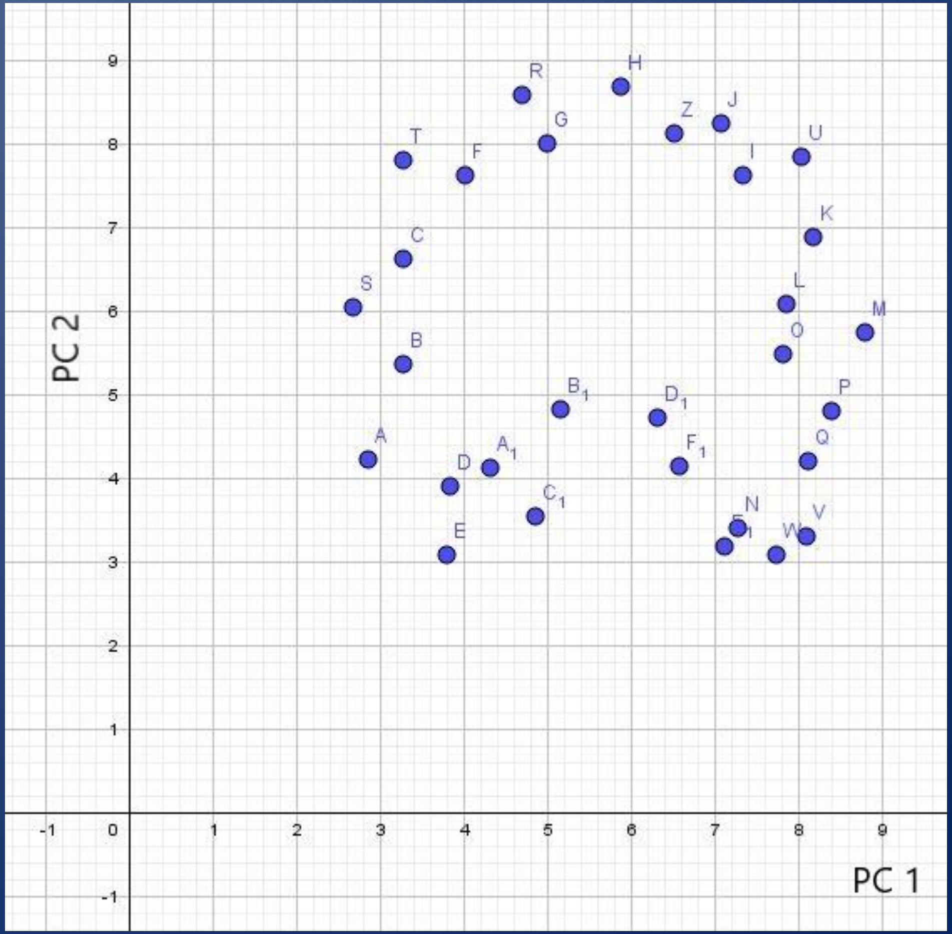
PCA is sensitive to outliers!

- Plot data set if possible

PRINCIPAL COMPONENTS ANALYSIS IMPORTANT REMARKS

<u>Horseshoe effect</u>

Example of „failure“ of PCA



PROJECT 3

CLUSTER SHAPE ANALYSIS