

# PCA, SVD and Other Related Acronyms

**Cristina España-Bonet**

UdS & DFKI, Saarbrücken, Germany

Summer Semester Seminar

15th May 2019

# The Problem

## *High Dimensional Data*

How do we deal with high dimensional data?

# The Problem

## High Dimensional Data

*time* = (1.844012, 0.590383, 1.003636, -0.577031, 1.515419, 1.097797, 1.812856, 0.933615, -2.396581, -0.931116, -0.719396, -0.376134, -1.204231, 0.045771, -0.287482, 1.084627, 4.399265, 1.516829, -0.838133, -1.881685, 0.108117, 2.345857, -1.292667, -2.286168, 3.419926, 4.260052, -1.016988, 3.140229, -3.161504, -0.800707, -1.433775, 2.290546, 1.932333, 0.714649, -3.033084, -0.958289, -1.704687, -1.597345, 1.525060, 3.337017, -2.787743, 1.479353, 3.452092, -3.242210, 0.532302, -0.551804, 2.344314, -0.919049, -1.872516, 0.080137, 1.208913, -2.136555, -2.218254, 0.206410, 0.133225, -1.521032, 1.735609, 2.885288, -2.048691, 2.375038, 0.316599, -0.254595, 2.159168, 1.118603, -0.775468, 0.933521, -0.351797, 2.193516, 2.499064, 2.818742, -0.213898, 0.446962, 1.767461, 1.342941, 1.117215, -0.042004, 4.199081, 3.041796, -1.770649, -0.528354, -2.067354, 0.283046, -0.099049, -0.105402, 2.823484, -2.583724, -2.906962, 0.592174, -3.029664, -0.170582, 0.406366, 1.963008, -3.229250, -3.499467, -0.136623, -1.551140, 0.348241, -1.597526, 0.703598, 3.122618, 0.466473, -0.113320, -2.119155, 1.092863, -0.908410, 0.253259, -1.082862, 4.408773, 2.419691, 2.343239, 0.703793, 1.270707, 0.410221, -1.293057, -0.799147, 2.214563, -0.212623, 1.206766, -0.731273, 2.308388, -1.029362, -2.080709, 0.749148, -1.412619, 1.073051, -2.498955, -0.520858, 1.391912, -1.181121, 1.523457, -1.245448, -0.290742, -2.589719, -0.366162, 3.586508, 0.908829, -1.125176, -0.937035, -1.163619, 1.759209, 3.678231, 0.019263, -0.395732, 1.142848, -0.500150, -3.005232, 2.287069, -0.524648, -0.944902, 0.038368, -1.093538, -0.697787, 0.767664, 2.399855, 2.425945, 1.563581, -1.086811, 0.372100, 1.400303, -2.278863, 0.643208, -0.459837, 1.756295, 2.057359, 3.140241, -1.740582, 1.386243, -1.822378, 1.528883, -1.984250, 1.214508, -1.336822, -0.321478, -0.162113, 0.272326, -2.673072, 0.612675, -0.657483, -0.557969, -3.358420, -2.559981, -1.683046, -1.314229, -2.425110, -2.506184, -1.606668, 1.332781, -2.760878, -2.400824, -1.830618, -2.406664, -1.169146, -1.838281, 0.588559, 2.285466, -0.401462, 1.632473, -0.510084, -2.072332, -2.627897, 2.531830, -2.524195, 2.035469, 1.906113, -1.257332, -4.039220, -0.467614, -2.275054, -3.409202, -0.014383, 0.445576, 1.461529, -1.318478, 0.061049, 0.280523, 2.173227, -0.027133, 2.791830, -0.728346, -1.804815, 1.245291, 0.970318, 2.646388, 0.246842, -1.823608, 1.888760, 0.265116, -2.027269, -0.089802, 0.389976, -0.654499, 2.565478, -2.647825, 2.658914, 1.385568, 2.306623, 0.476923, -0.869644, -0.170338, 0.495097, -2.604649, 0.610231, 0.739677, 0.322778, -2.042915, -1.353154, 0.177016, 1.840185, -0.271689, -0.401560, -0.421108, -0.185526, 1.041765, -4.599578, -0.829409, 0.076258, -0.503421, 1.891007, -0.931777, 0.434825, -0.467926, -1.417658, -0.320597, -4.084039, -3.899607, 0.977403, 0.774670, 3.269479, -1.031264, -0.433907, -2.305760, 0.811788, 2.347483, -1.254061, -0.861366, 0.080974, -3.666142, -0.363376, -2.384475, -4.290071, -0.924723, 1.257435, 1.223927, 0.276726, 1.541471, 1.274240, 1.883040, -1.987514, -0.809325, 1.252716, 1.812783, -0.511801, -1.657522, 1.196169, 0.804855, -1.861488, -2.113367, 0.429888, -0.920844, 0.377247)

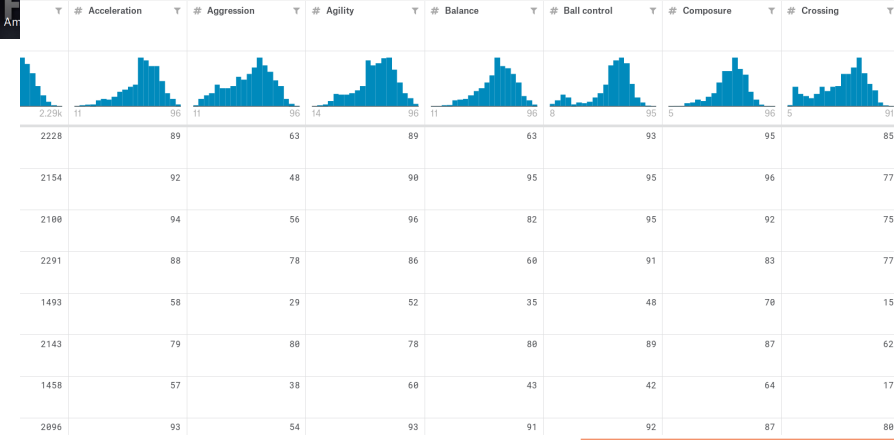
# The Problem

## High Dimensional Data

Dataset Released Under CC BY-NC-SA 4.0

### FIFA 18 Complete Player Dataset

17k+ players, 70+ attributes extracted from the latest edition of FIFA



# The Problem

## *High Dimensional Data*

How do we deal with high dimensional data?

- Are all dimensions relevant?
- Are they correlated?
- All of them describe the data?

# The Problem

## *High Dimensional Data*

How do we deal with high dimensional data?

- Are all dimensions relevant?
- Are they correlated?
- All of them describe the data?

These questions are related to **feature selection**, **data compression**, **visualisation**...

# The Problem

## *High Dimensional Data*

How do we deal with high dimensional data?

- Are all dimensions relevant?
- Are they correlated?
- All of them describe the data?

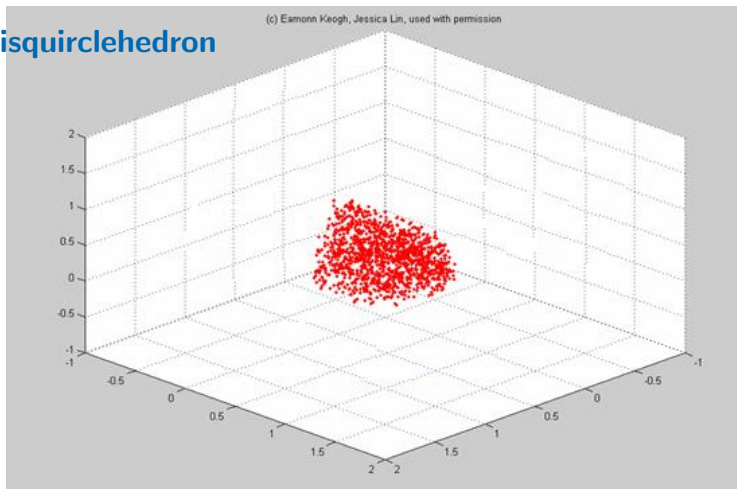
These questions are related to **feature selection**, **data compression**, **visualisation**...

Let's **project** into a lower dimensional space, but **wisely**...

# The Problem

*Is any kind of projection valid?*

## Trisquirlehedron



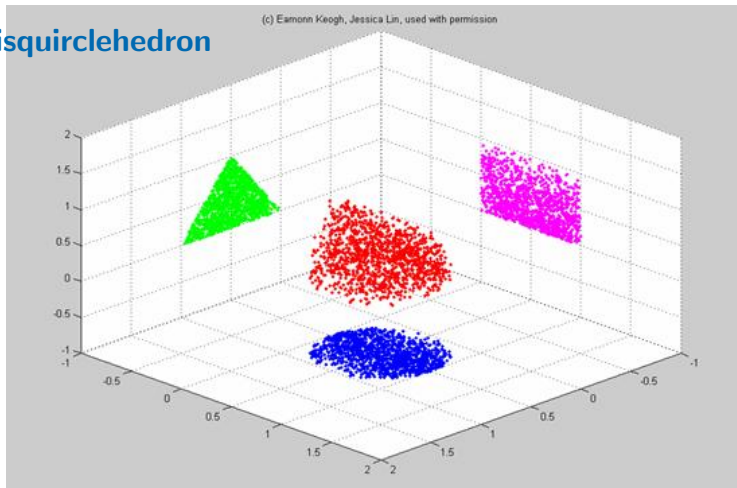
<https://cs.gmu.edu/~jessica/DimReducDanger.htm>



# The Problem

*Is any kind of projection valid?*

## Trisquirlehedron



<https://cs.gmu.edu/~jessica/DimReducDanger.htm>

The Problem

*A Solution*

# Principal Component Analysis

# Outline

- 1 Introduction
- 2 Principal Component Analysis, PCA
- 3 Singular-Value Decomposition, SVD
- 4 Comments & Final Remarks

# Introduction

## *Outline*

- 1 Introduction
- 2 Principal Component Analysis, PCA
- 3 Singular-Value Decomposition, SVD
- 4 Comments & Final Remarks

# Introduction

## *Principal Component Analysis (PCA)*

### **Description:**

Linear projection of a set of data points from a space defined by many correlated variables into a space defined by fewer uncorrelated coordinates called principal components while still retaining most of the variability present in the data.

# Introduction

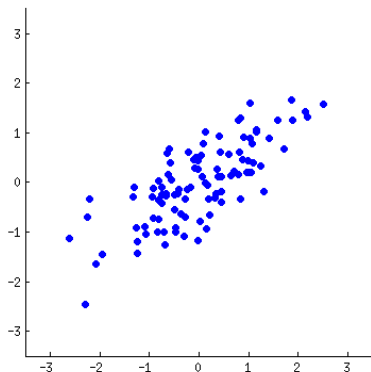
## *Principal Component Analysis (PCA)*

### Description:

**Linear** projection of a set of data points from a space defined by many correlated variables into a space defined by fewer **uncorrelated** coordinates called principal components while still retaining most of the **variability** present in the data.

# Introduction

## *PCA: Visualisation in $2D \Rightarrow 1D$*

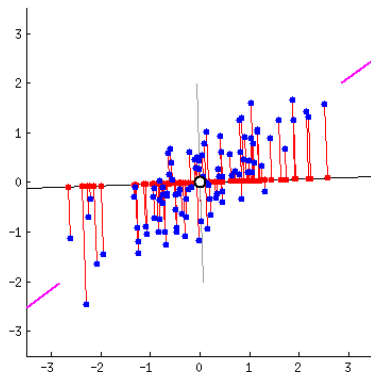


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*



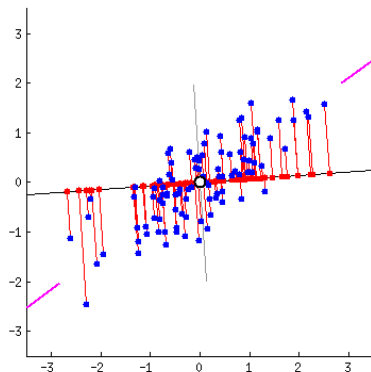
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)



# Introduction

## *PCA: Visualisation*

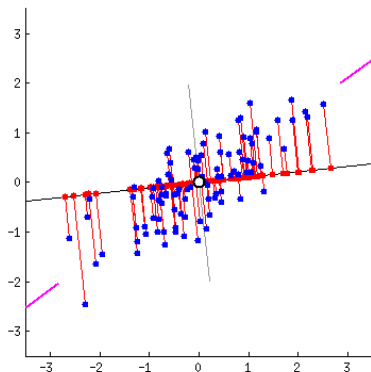


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

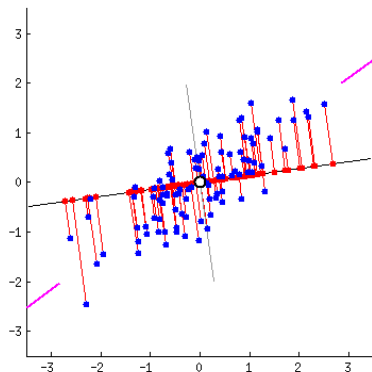


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

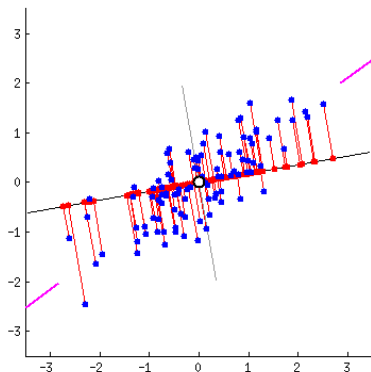


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

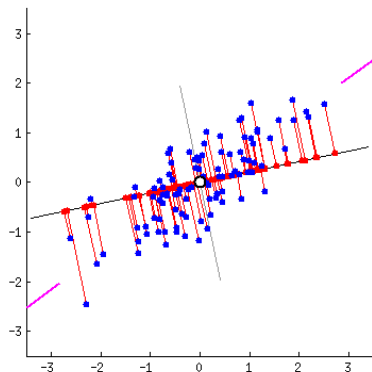


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

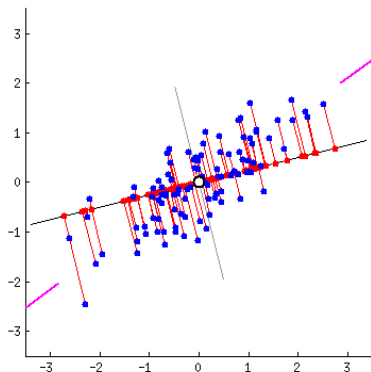


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

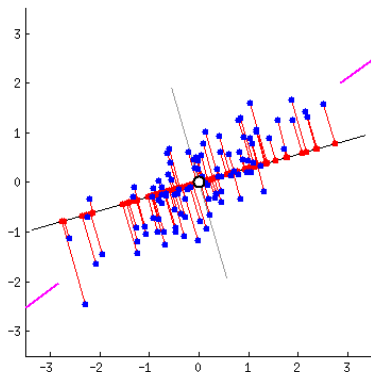


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

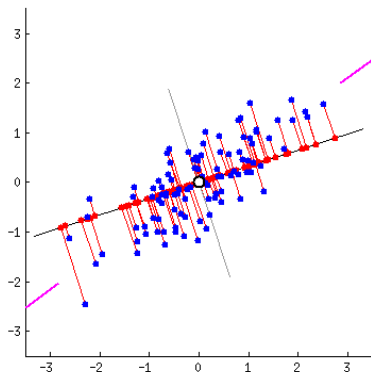


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



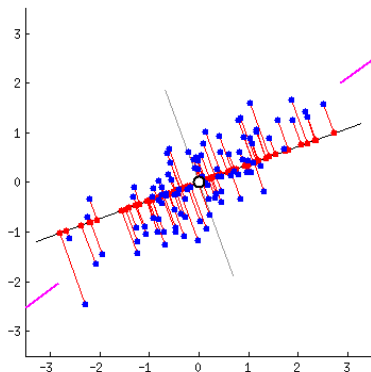
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)



# Introduction

## *PCA: Visualisation*

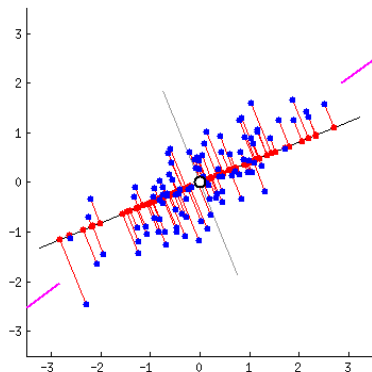


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

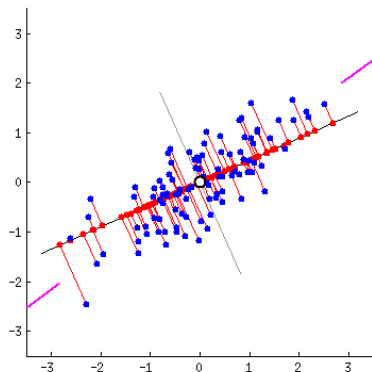


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

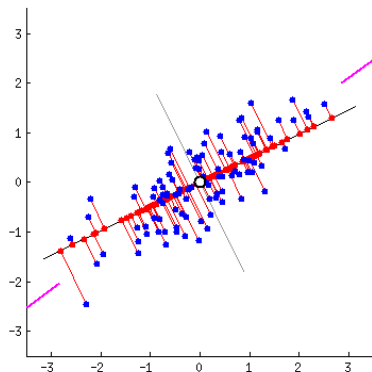


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

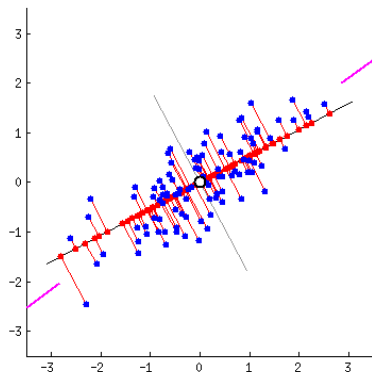


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

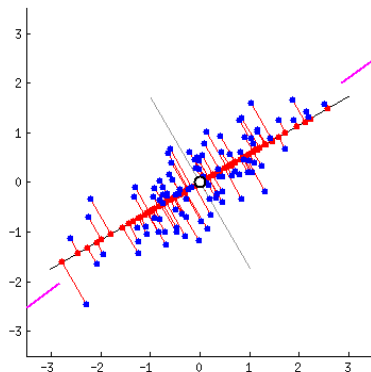


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

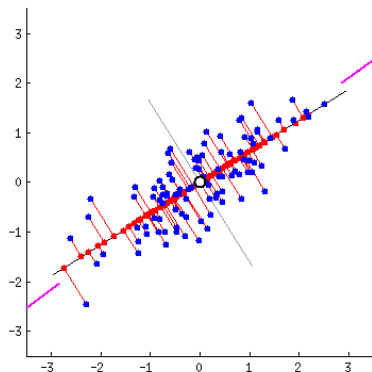


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

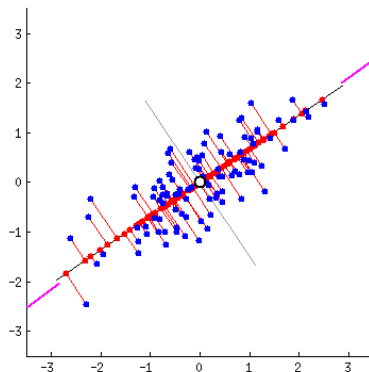


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*



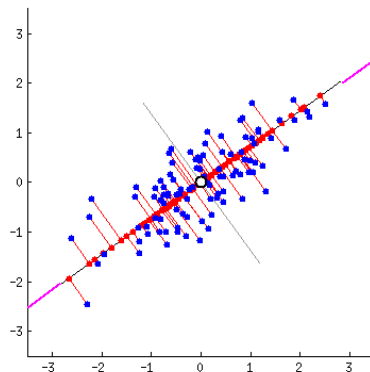
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)



# Introduction

## *PCA: Visualisation*

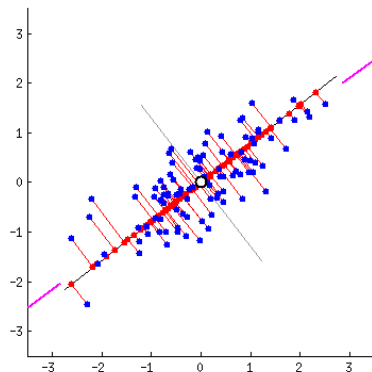


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

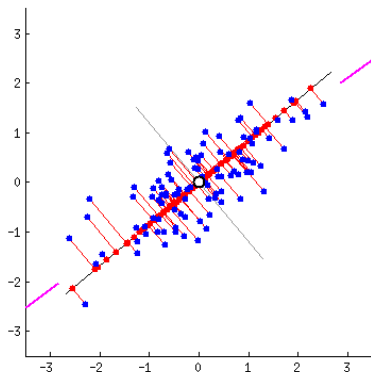


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

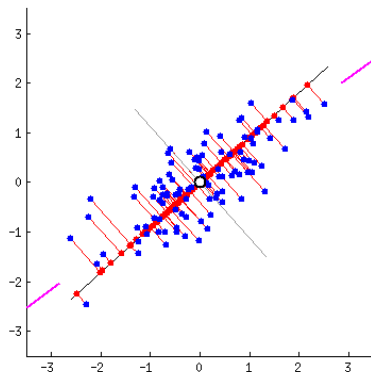


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

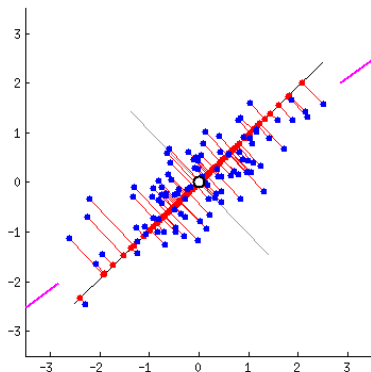


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

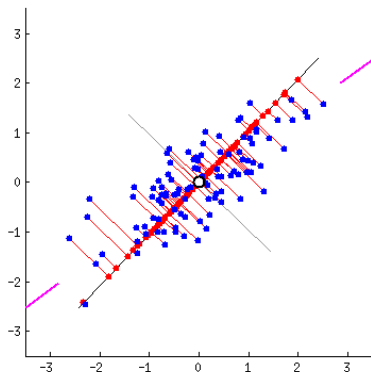


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

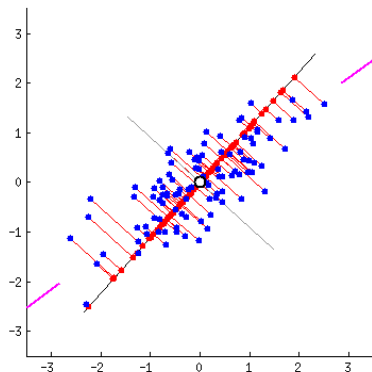


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

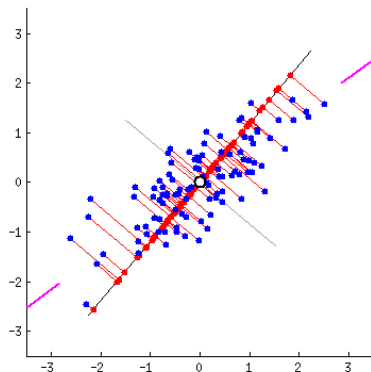


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



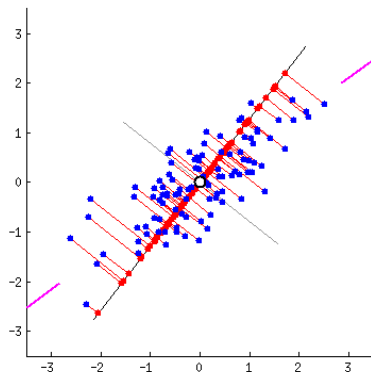
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)



# Introduction

## *PCA: Visualisation*

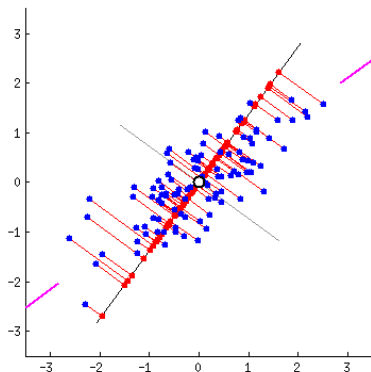


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

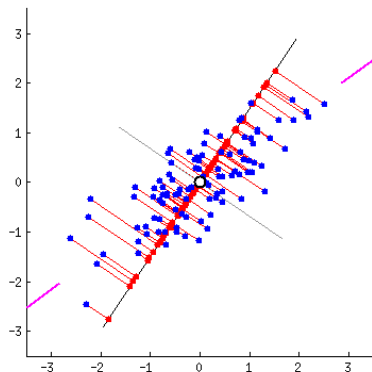


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

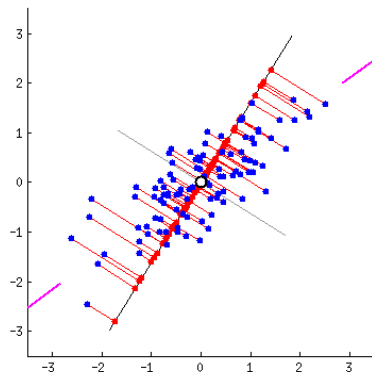


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

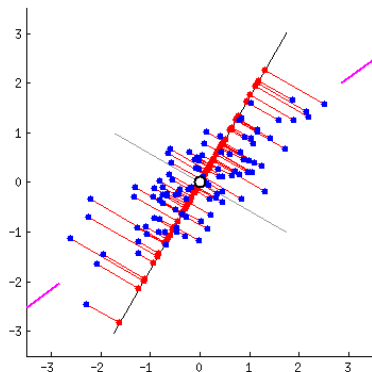


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

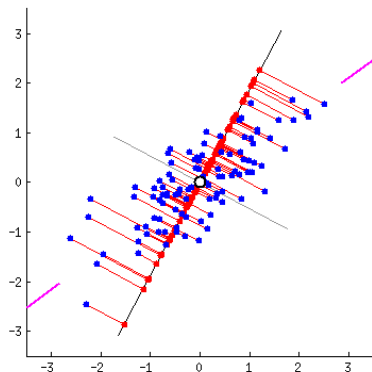


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

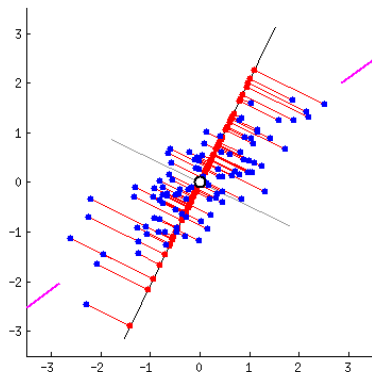


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

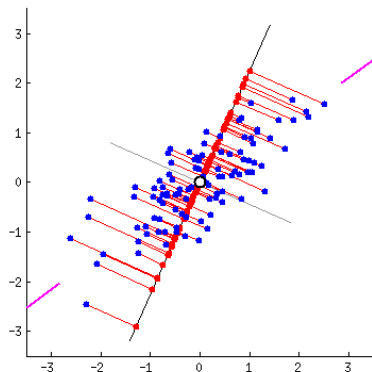


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



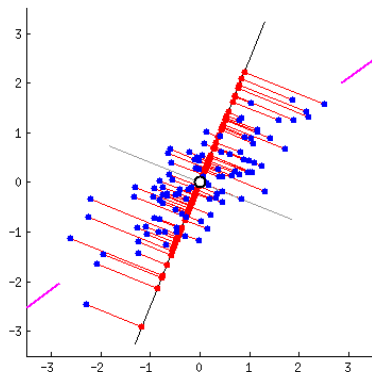
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)



# Introduction

## *PCA: Visualisation*

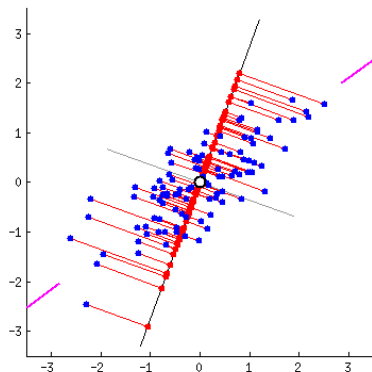


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

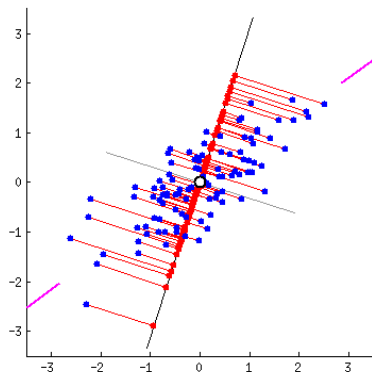


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

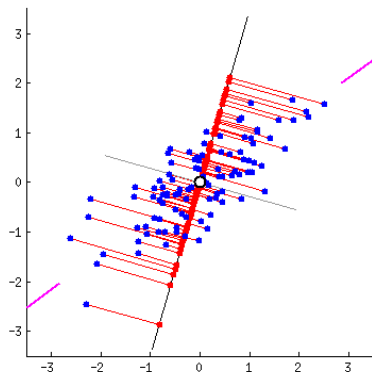


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

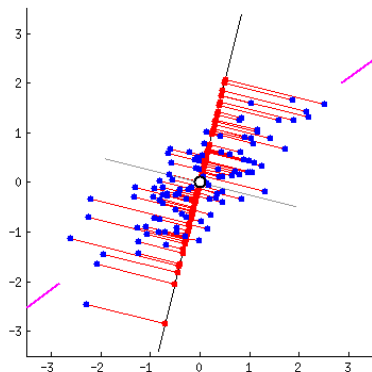


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

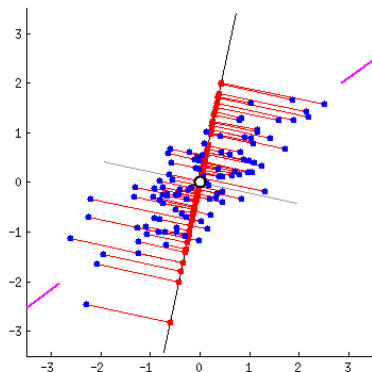


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

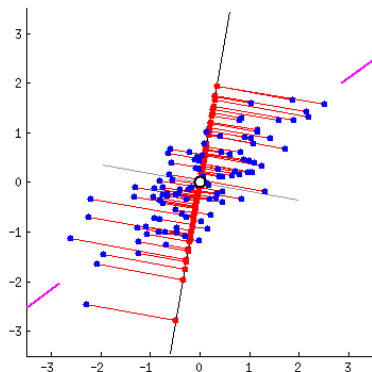


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

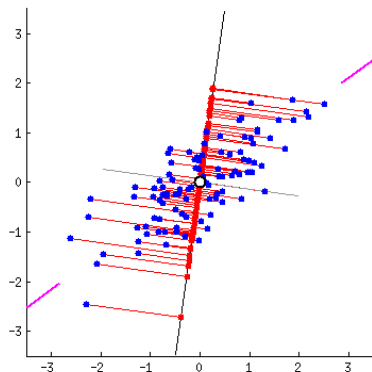


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



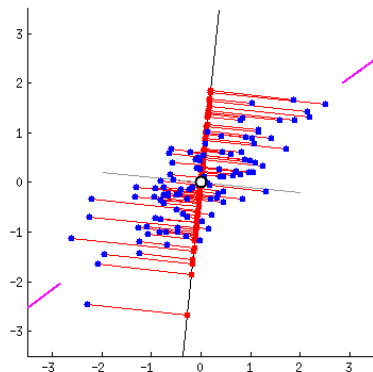
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)



# Introduction

## *PCA: Visualisation*

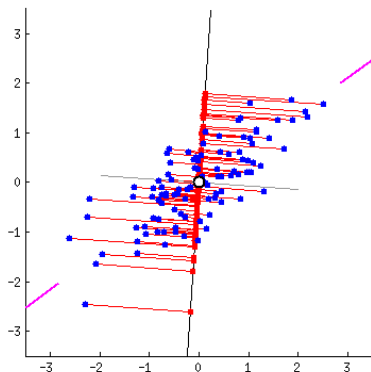


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

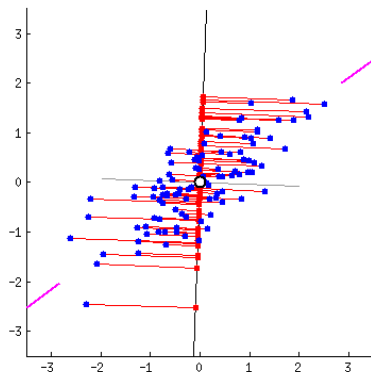


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

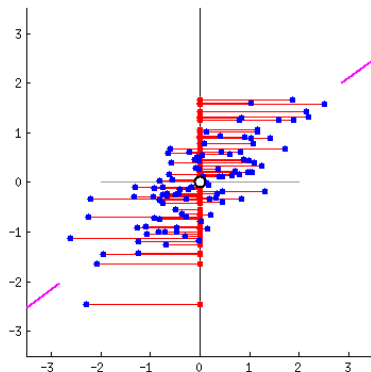


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

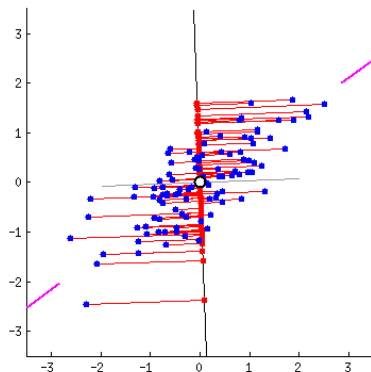


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

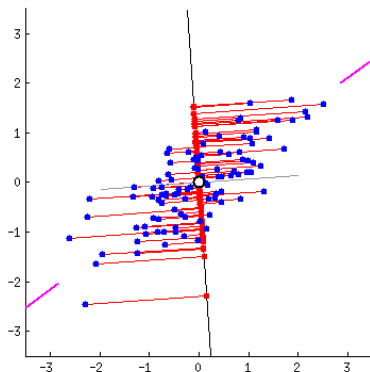


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

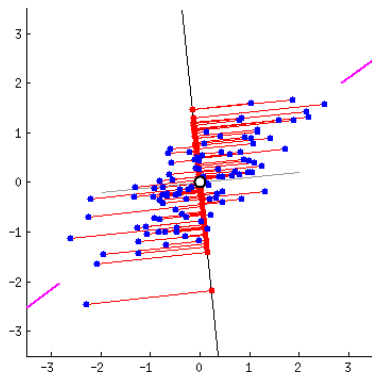


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

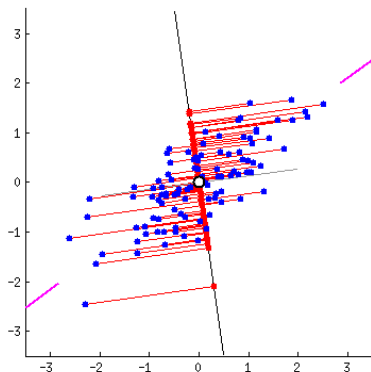


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



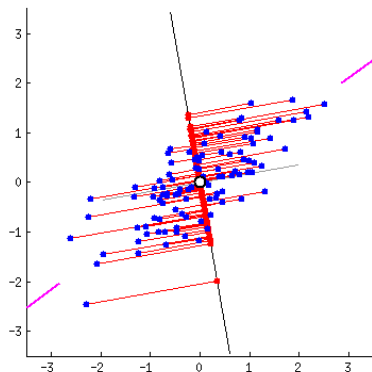
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)



# Introduction

## *PCA: Visualisation*

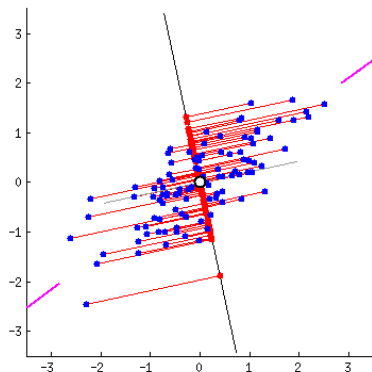


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

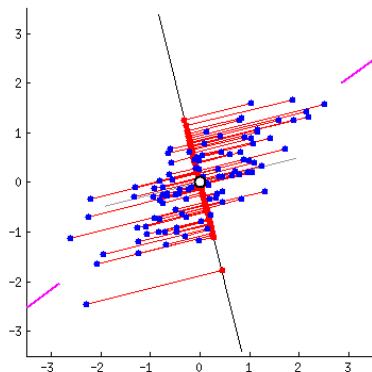


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

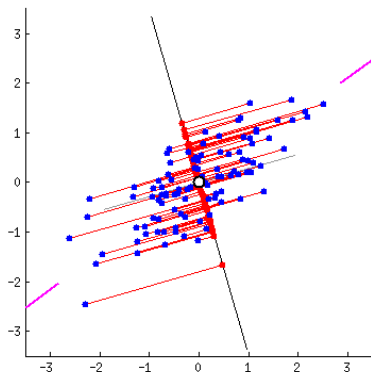


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

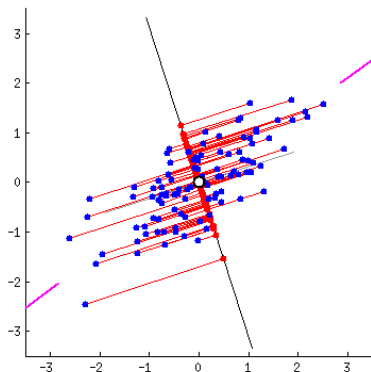


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

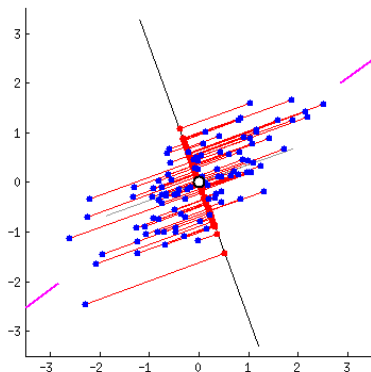


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

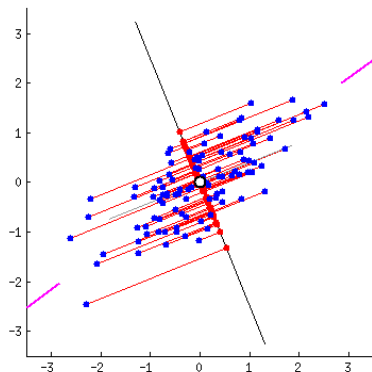


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

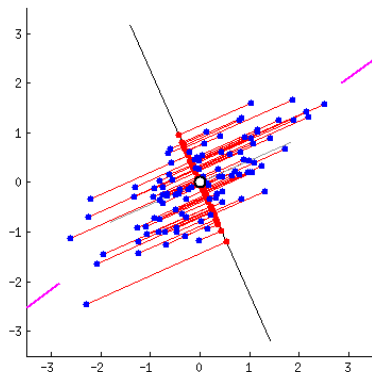


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



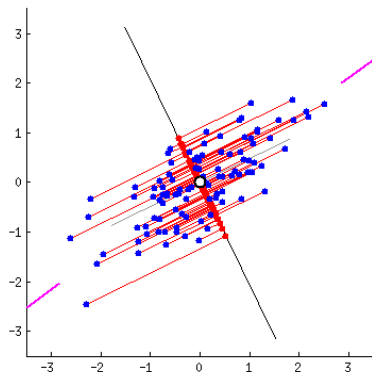
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)



# Introduction

## *PCA: Visualisation*

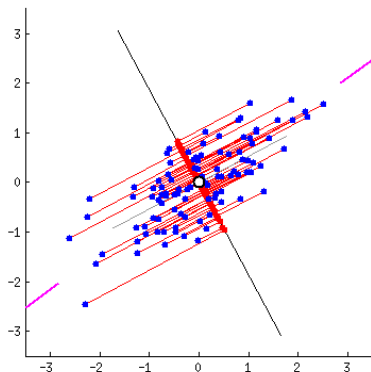


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

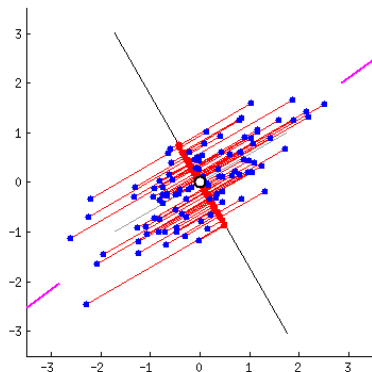


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

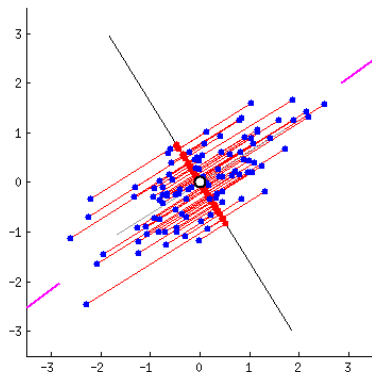


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

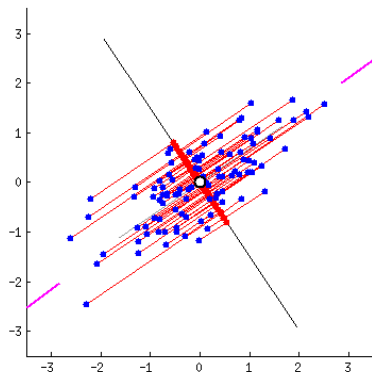


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

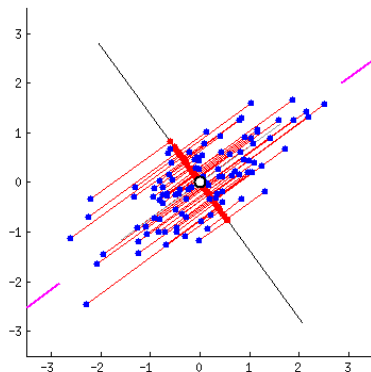


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

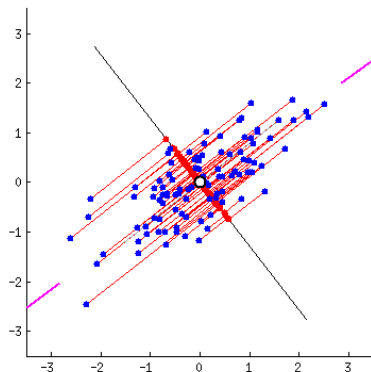


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

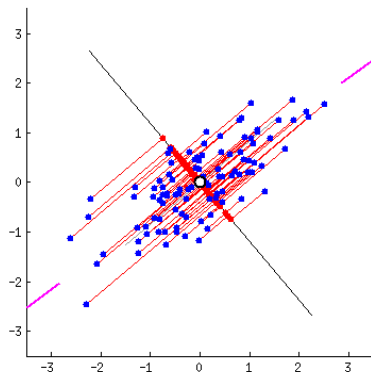


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



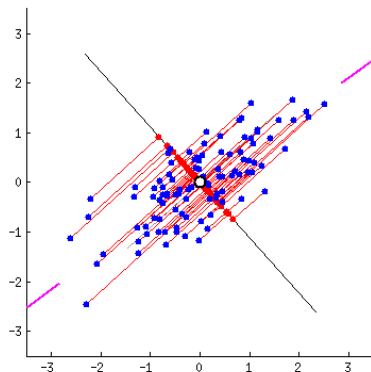
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)



# Introduction

## *PCA: Visualisation*

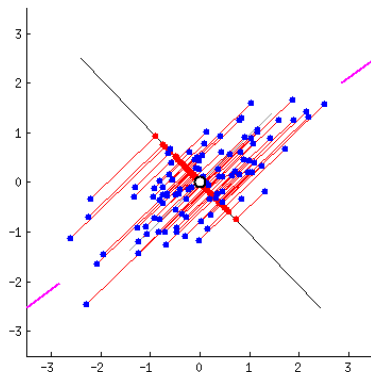


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

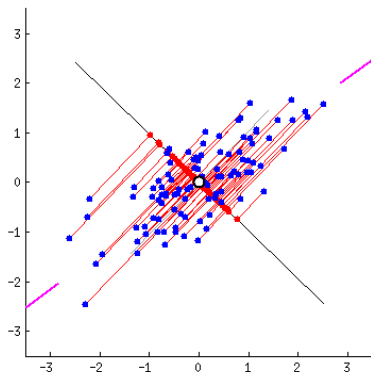


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

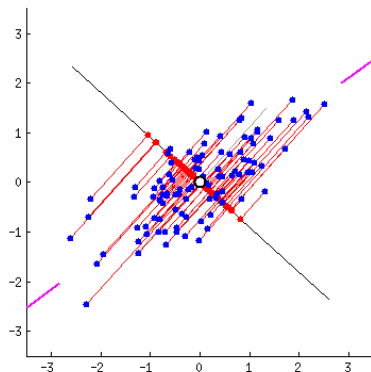


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

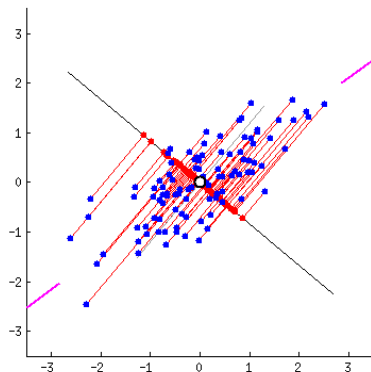


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

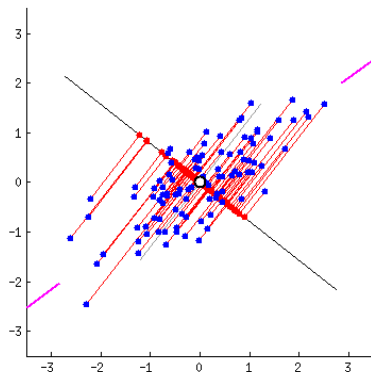


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

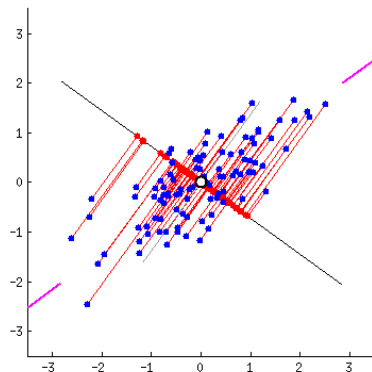


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

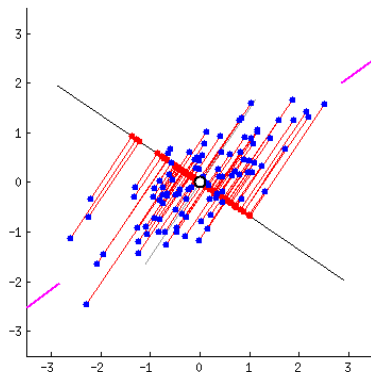
## *PCA: Visualisation*



[https://stats.stackexchange.com/questions/2691/  
/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*



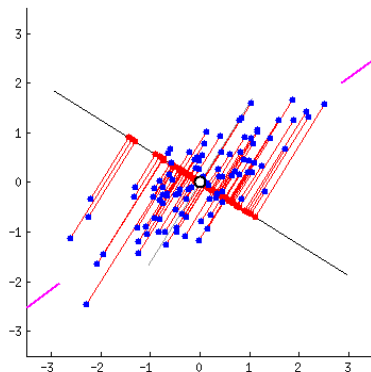
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)



# Introduction

## *PCA: Visualisation*

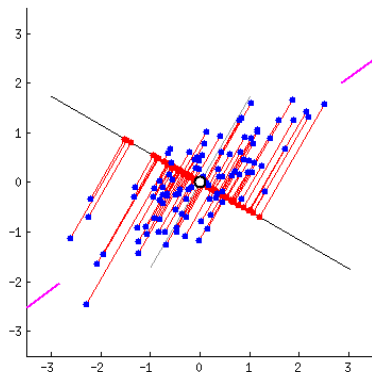


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

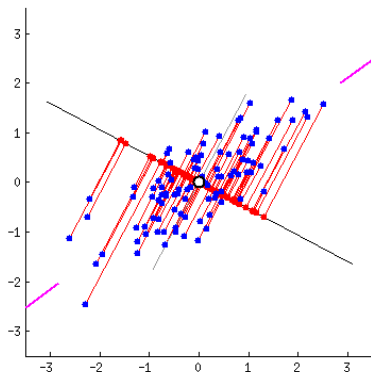


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

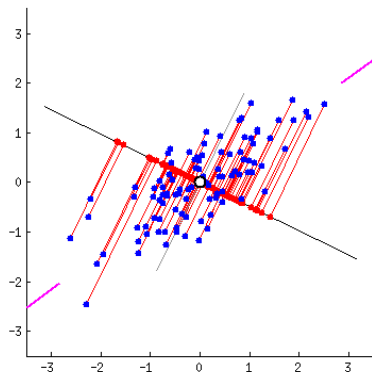


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

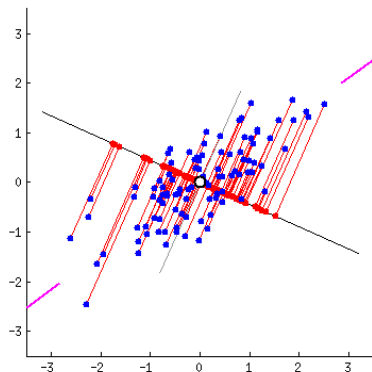


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

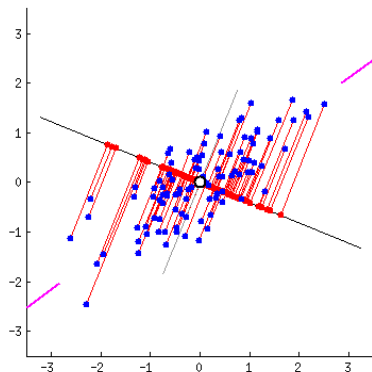


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

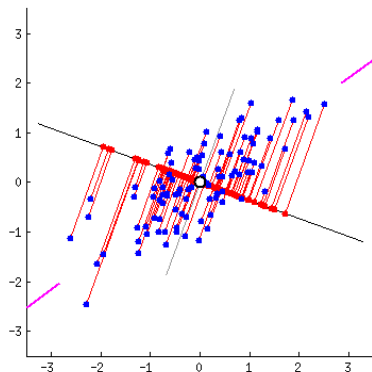


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

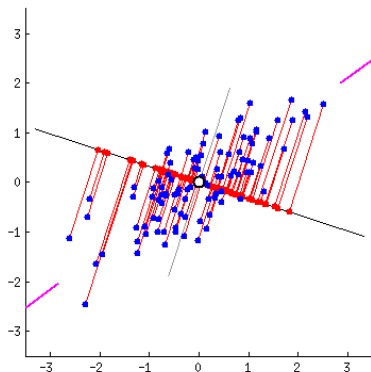


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*



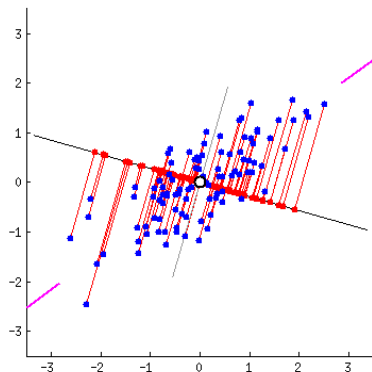
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)



# Introduction

## *PCA: Visualisation*

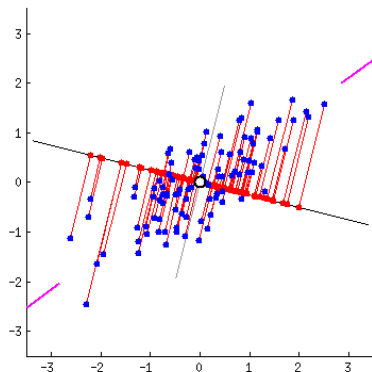


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

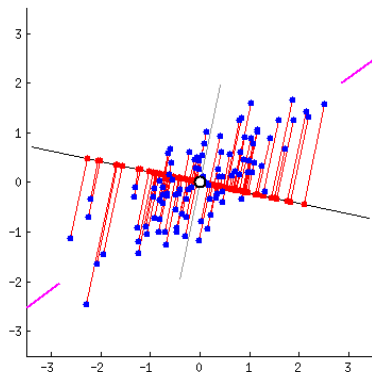


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

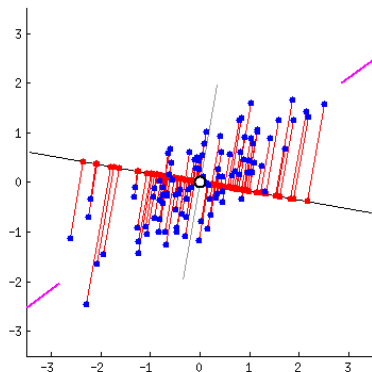


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Introduction

## *PCA: Visualisation*

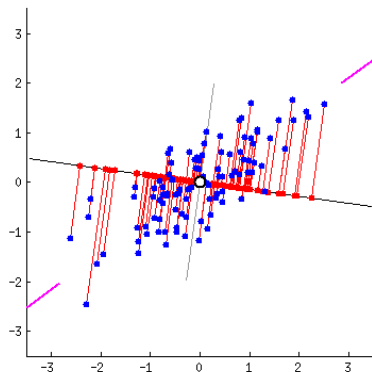


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

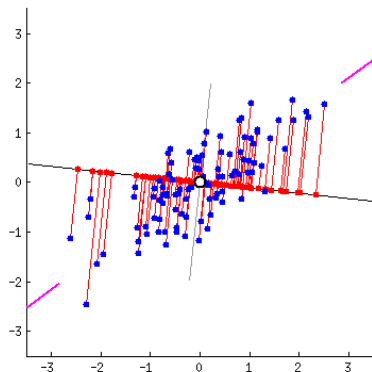


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

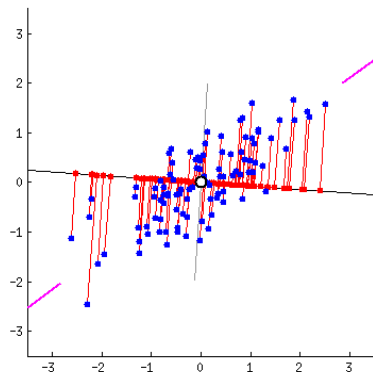


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*

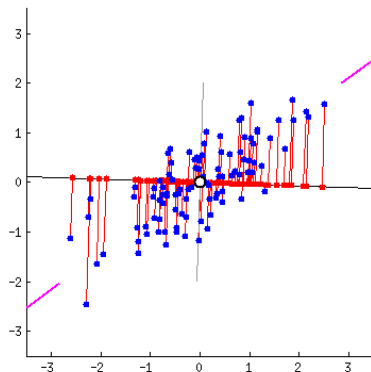


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)

# Introduction

## *PCA: Visualisation*



<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/)



# Introduction

## *PCA: Usages*

- Dimensionality reduction/projection
  - Compression, clustering, classification...
- Orthogonalisation of the dimensions
  - Input for other algorithms
- Visualisation
- Data interpretation
  - Feature selection
- ...

# Introduction

## *PCA: How?*

- 1 Eigenvalue decomposition of a data covariance matrix
- 2 Singular value decomposition of a data matrix

# Principal Component Analysis, PCA

## *Outline*

- 1 Introduction
- 2 Principal Component Analysis, PCA
- 3 Singular-Value Decomposition, SVD
- 4 Comments & Final Remarks

# Principal Component Analysis, PCA

## *Eigenvectors and Eigenvalues*

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

Eigenvectors  $\mathbf{v}$  and eigenvalues  $\lambda$  of a matrix  $\mathbf{A}$

# Principal Component Analysis, PCA

## *Eigenvectors and Eigenvalues*

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

Eigenvectors  $\mathbf{v}$  and eigenvalues  $\lambda$  of a matrix  $\mathbf{A}$

For a given  $\mathbf{A}$ , how do we obtain them?

$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0$ , where  $\mathbf{I}$  is the identity matrix

# Principal Component Analysis, PCA

## *Eigenvectors and Eigenvalues*

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

Eigenvectors  $\mathbf{v}$  and eigenvalues  $\lambda$  of a matrix  $\mathbf{A}$

For a given  $\mathbf{A}$ , how do we obtain them?

$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0$ , where  $\mathbf{I}$  is the identity matrix

1. **Eigenvalues**  $|\mathbf{A} - \lambda\mathbf{I}| = 0 \Rightarrow \lambda_i$

2. **Eigenvectors**  $(\mathbf{A} - \lambda_i\mathbf{I})\mathbf{v}_{\lambda_i} = 0 \Rightarrow \mathbf{v}_{\lambda_i}$

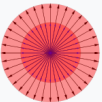
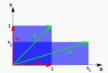
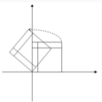
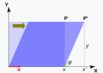
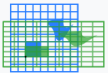
# Principal Component Analysis, PCA

## *Eigenvectors and Eigenvalues*

<b>Matrix</b>	$\begin{bmatrix} k & 0 \\ 0 & k \end{bmatrix}$	$\begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix}$	$\begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ $c = \cos \theta$ $s = \sin \theta$	$\begin{bmatrix} 1 & k \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} c & s \\ s & c \end{bmatrix}$ $c = \cosh \varphi$ $s = \sinh \varphi$
---------------	--	--	---	--	--

# Principal Component Analysis, PCA

## *Eigenvectors and Eigenvalues*

	Scaling	Unequal scaling	Rotation	Horizontal shear	Hyperbolic rotation
<b>Illustration</b>					
<b>Matrix</b>	$\begin{bmatrix} k & 0 \\ 0 & k \end{bmatrix}$	$\begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix}$	$\begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ $c = \cos \theta$ $s = \sin \theta$	$\begin{bmatrix} 1 & k \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} c & s \\ s & c \end{bmatrix}$ $c = \cosh \varphi$ $s = \sinh \varphi$
<b>Characteristic polynomial</b>	$(\lambda - k)^2$	$(\lambda - k_1)(\lambda - k_2)$	$\lambda^2 - 2c\lambda + 1$	$(\lambda - 1)^2$	$\lambda^2 - 2c\lambda + 1$
<b>Eigenvalues, <math>\lambda_i</math></b>	$\lambda_1 = \lambda_2 = k$	$\lambda_1 = k_1$ $\lambda_2 = k_2$	$\lambda_1 = e^{i\theta} = c + s\mathbf{i}$ $\lambda_2 = e^{-i\theta} = c - s\mathbf{i}$	$\lambda_1 = \lambda_2 = 1$	$\lambda_1 = e^{\varphi}$ $\lambda_2 = e^{-\varphi}$
<b>Eigenvectors</b>	All non-zero vectors	$u_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $u_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$u_1 = \begin{bmatrix} 1 \\ -\mathbf{i} \end{bmatrix}$ $u_2 = \begin{bmatrix} 1 \\ +\mathbf{i} \end{bmatrix}$	$u_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$	$u_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $u_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$



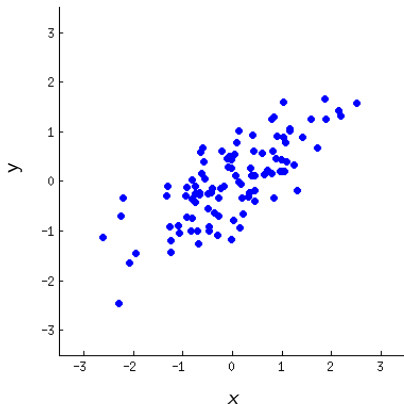
# Principal Component Analysis, PCA

## *PCA: How?*

- 1 Eigenvalue decomposition of a data **covariance matrix**
- 2 Singular value decomposition of a data matrix

# Principal Component Analysis, PCA

## *Covariance Matrix*

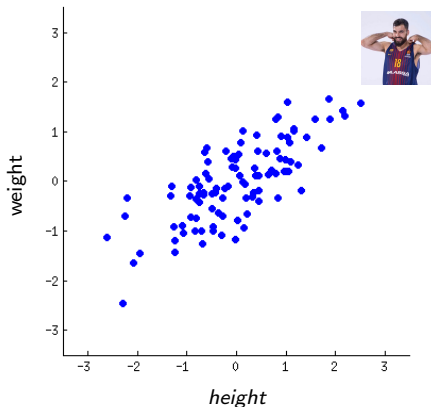


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Principal Component Analysis, PCA

## *Covariance Matrix*

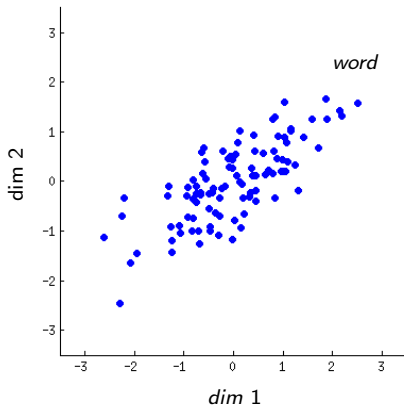


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](#)

# Principal Component Analysis, PCA

## *Covariance Matrix*

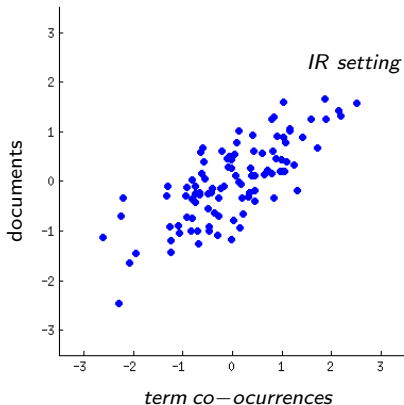


<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

# Principal Component Analysis, PCA

## *Covariance Matrix*



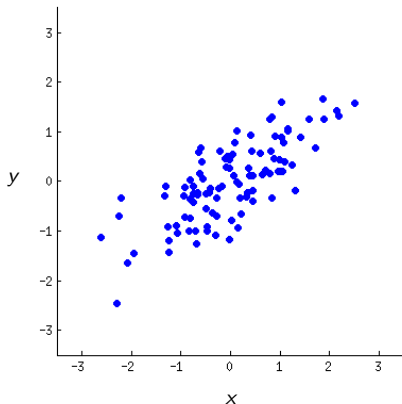
<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](#)

# Principal Component Analysis, PCA

## Covariance Matrix

$$\mu_x = \frac{1}{n} \sum_{i=1}^n x_i, \quad \mu_y = \frac{1}{n} \sum_{i=1}^n y_i$$



<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues)

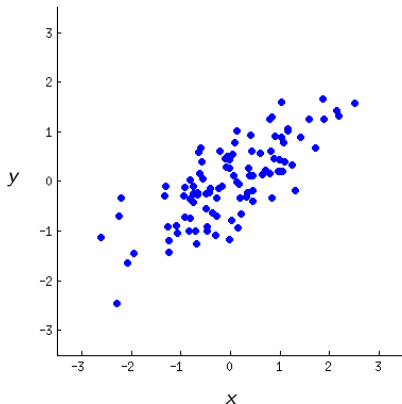
# Principal Component Analysis, PCA

## Covariance Matrix

$$\mu_x = \frac{1}{n} \sum_{i=1}^n x_i, \quad \mu_y = \frac{1}{n} \sum_{i=1}^n y_i$$

$$\sigma_x^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \mu_x)^2 = \text{var}(x)$$

$$\begin{aligned} \sigma_{xy}^2 &= \frac{1}{n-1} \sum_{i=1}^n (x_i - \mu_x)(y_i - \mu_y) \\ &= \text{covar}(x, y) \end{aligned}$$



<https://stats.stackexchange.com/questions/2691/>

[/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues](#)

# Principal Component Analysis, PCA

*Covariance Matrix,  $\Sigma$*

$$\text{In 2D, } \Sigma = \begin{pmatrix} \sigma_{xx}^2 & \sigma_{yx}^2 \\ \sigma_{xy}^2 & \sigma_{yy}^2 \end{pmatrix} \quad \text{with } \sigma_{xy}^2 = \sigma_{yx}^2,$$



# Principal Component Analysis, PCA

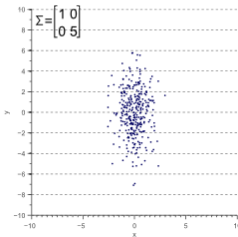
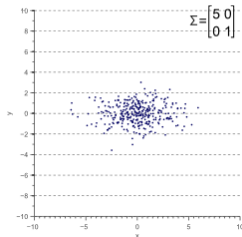
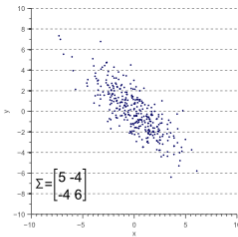
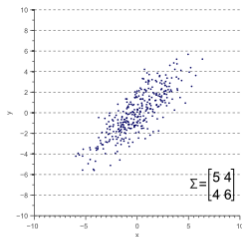
## Covariance Matrix, $\Sigma$

$$\text{In 2D, } \Sigma = \begin{pmatrix} \sigma_{xx}^2 & \sigma_{yx}^2 \\ \sigma_{xy}^2 & \sigma_{yy}^2 \end{pmatrix} \quad \text{with } \sigma_{xy}^2 = \sigma_{yx}^2,$$

$$\text{In general, } \Sigma = \begin{pmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 & \cdots & \sigma_{1n}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 & \cdots & \sigma_{2n}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & \sigma_{33}^2 & \cdots & \sigma_{3n}^2 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \sigma_{n1}^2 & \sigma_{n2}^2 & \sigma_{n3}^2 & \cdots & \sigma_{nn}^2 \end{pmatrix}$$

# Principal Component Analysis, PCA

## Covariance Matrix, $\Sigma$



# Principal Component Analysis, PCA

## *Principal Components and Maximum Variance*

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

What do we want?

# Principal Component Analysis, PCA

## *Principal Components and Maximum Variance*

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

What do we want?

- 1 Project  $\mathbf{x}$  into an  $\mathbf{x}'$  with maximum variance
- 2  $\mathbf{x}'$  (with  $\mathbf{y}'$ ,  $\mathbf{z}'$ ...) to be orthogonal

# Principal Component Analysis, PCA

## *Principal Components and Maximum Variance*

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

What do we want?

- 1 Project  $\mathbf{x}$  into an  $\mathbf{x}'$  with maximum variance
  - projection of  $\mathbf{x}$  is  $\mathbf{x}' = \mathbf{v}^T \mathbf{x}$
- 2  $\mathbf{x}'$  (with  $\mathbf{y}'$ ,  $\mathbf{z}'$ ...) to be orthogonal
  - constraint  $\|\mathbf{v}\| = \mathbf{v}^T \mathbf{v} = 1$

# Principal Component Analysis, PCA

## *Principal Components and Maximum Variance*

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

What do we want?

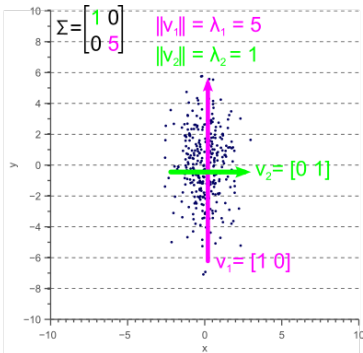
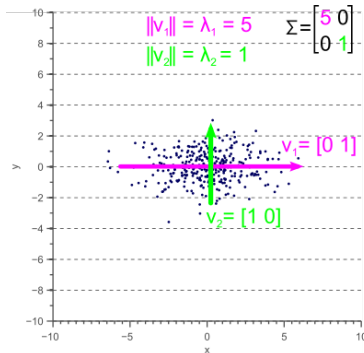
- 1 Project  $\mathbf{x}$  into an  $\mathbf{x}'$  with maximum variance
  - projection of  $\mathbf{x}$  is  $\mathbf{x}' = \mathbf{v}^T \mathbf{x}$
- 2  $\mathbf{x}'$  (with  $\mathbf{y}'$ ,  $\mathbf{z}'$ ...) to be orthogonal
  - constraint  $\|\mathbf{v}\| = \mathbf{v}^T \mathbf{v} = 1$

Some linear algebra and Lagrange multipliers later...

$$\mathbf{\Sigma} \mathbf{v} = \lambda \mathbf{v}$$

# Principal Component Analysis, PCA

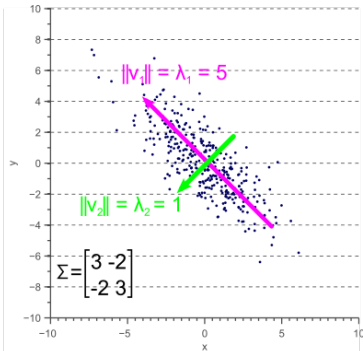
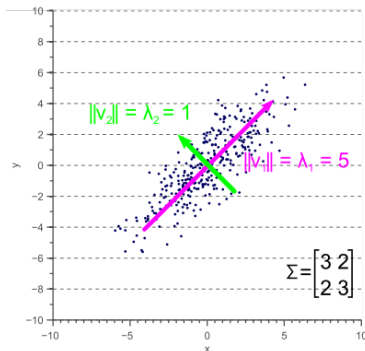
## Principal Components



<http://www.visiondummy.com/2014/04/geometric-interpretation-covariance-matrix/>

# Principal Component Analysis, PCA

## Principal Components



<http://www.visiondummy.com/2014/04/geometric-interpretation-covariance-matrix/>



# Principal Component Analysis, PCA

## *PCA: How?*

- 1 Eigenvalue decomposition of a data covariance matrix
- 2 Singular value decomposition of a data matrix

# Principal Component Analysis, PCA

## *Eigenvalue Decomposition Method, Wrap Up*

- 1 Eigenvalue decomposition of a data covariance matrix
  - Center (or standardise) the data
  - Calculate the covariance matrix
  - Calculate its eigenvalues
  - Rank the eigenvalues
  - Take the top- $k$  to get the new  $k$  uncorrelated dimensions

# Principal Component Analysis, PCA

## *Eigenvalue Decomposition Method, Wrap Up*

- 1 Eigenvalue decomposition of a data covariance matrix
  - Center (or standardise) the data
  - Calculate the covariance matrix
  - Calculate its eigenvalues
  - Rank the eigenvalues
  - Take the top- $k$  to get the new  $k$  uncorrelated dimensions

Is this *pca.fit\_transform(x)*?

- Numerically unstable

# Principal Component Analysis, PCA

## *Eigenvalue Decomposition Method, Wrap Up*

- 1 Eigenvalue decomposition of a data covariance matrix
  - Center (or standardise) the data
  - Calculate the covariance matrix
  - Calculate its eigenvalues
  - Rank the eigenvalues
  - Take the top- $k$  to get the new  $k$  uncorrelated dimensions

Is this *pca.fit\_transform(x)*?

- Numerically unstable
- 2 Singular value decomposition of a data matrix

# Singular-Value Decomposition, SVD

## *Outline*

- 1 Introduction
- 2 Principal Component Analysis, PCA
- 3 Singular-Value Decomposition, SVD**
- 4 Comments & Final Remarks

# Singular-Value Decomposition, SVD

## *Basics*

- Linear algebra

# Singular-Value Decomposition, SVD

## *Basics*

- Linear algebra
- **Factorisation** of a matrix  $\mathbf{A}$  as  $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$

# Singular-Value Decomposition, SVD

## *Basics*

- Linear algebra
- **Factorisation** of a matrix **A** as **A** = **USV**<sup>T</sup>
  - ✓ **U** is an  $m \times m$  orthogonal matrix,



# Singular-Value Decomposition, SVD

## Basics

- Linear algebra
- **Factorisation** of a matrix **A** as **A** = **USV**<sup>T</sup>
  - ✓ **U** is an  $m \times m$  **orthogonal matrix**,
    - $\mathbf{U}^T \mathbf{U} = \mathbf{U} \mathbf{U}^T = \mathbf{I}$
    - or, equivalently,  $\mathbf{U}^T = \mathbf{U}^{-1}$

# Singular-Value Decomposition, SVD

## Basics

- Linear algebra
- **Factorisation** of a matrix  $\mathbf{A}$  as  $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$ 
  - ✓  $\mathbf{U}$  is an  $m \times m$  orthogonal matrix,
  - ✓  $\mathbf{S}$  is a diagonal  $m \times n$  matrix with non-negative real numbers,

# Singular-Value Decomposition, SVD

## Basics

- Linear algebra
- **Factorisation** of a matrix **A** as **A** = **USV<sup>T</sup>**
  - ✓ **U** is an  $m \times m$  orthogonal matrix,
  - ✓ **S** is a diagonal  $m \times n$  matrix with non-negative real numbers,
  - ✓ **V<sup>T</sup>** is the conjugate transpose of an  $n \times n$  orthogonal matrix

# Singular-Value Decomposition, SVD

## Basics

$$\begin{pmatrix} m \times n \end{pmatrix} = \begin{pmatrix} m \times m \end{pmatrix} \begin{pmatrix} m \times n \end{pmatrix} \begin{pmatrix} n \times n \end{pmatrix}$$

$$\mathbf{A} = \mathbf{U} \mathbf{S} \mathbf{V}^T$$

# Singular-Value Decomposition, SVD

## *SVD: Singular Values*

$$\mathbf{S} = \begin{pmatrix} s_1 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \ddots \\ 0 & & & & s_r \\ & & & & & 0 \end{pmatrix};$$

$s_1 \dots s_r$ , singular values of  $\mathbf{A}$  (in decreasing order)

$r$ , rank of  $\mathbf{A}$

# Singular-Value Decomposition, SVD

## *SVD: Singular Values*

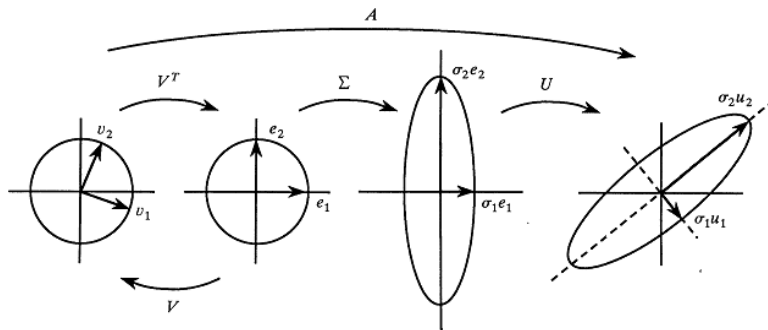
$$\mathbf{S} = \begin{pmatrix} s_1 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \ddots \\ 0 & & & & s_r \\ & & & & & 0 \end{pmatrix}; \quad \mathbf{A}_r = \sum_{i=1}^r s_i \vec{u}_i \vec{v}_i^T$$

$s_1 \dots s_r$ , singular values of  $\mathbf{A}$  (in decreasing order)

$r$ , rank of  $\mathbf{A}$

# Singular-Value Decomposition, SVD

## SVD: $2 \times 2$ Geometric Interpretation



$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$ : a linear transformation is a rotation or reflection, followed by a scaling, followed by another rotation or reflection

# Singular-Value Decomposition, SVD

## *Relation with Eigenvalue Decomposition*

Data  $\mathbf{X}$  (is now our  $\mathbf{A}$ ),      Data Covariance  $\mathbf{\Sigma} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$   
 $\mathbf{X} = \mathbf{USV}^T$



# Singular-Value Decomposition, SVD

## *Relation with Eigenvalue Decomposition*

Data  $\mathbf{X}$  (is now our  $\mathbf{A}$ ),      Data Covariance  $\mathbf{\Sigma} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$   
 $\mathbf{X} = \mathbf{USV}^T$

Let's SVD-decompose the data and estimate the covariance:

$$\mathbf{\Sigma} = \frac{1}{n-1}(\mathbf{USV}^T)^T(\mathbf{USV}^T)$$

# Singular-Value Decomposition, SVD

## *Relation with Eigenvalue Decomposition*

Data  $\mathbf{X}$  (is now our  $\mathbf{A}$ ),      Data Covariance  $\mathbf{\Sigma} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$   
 $\mathbf{X} = \mathbf{USV}^T$

Let's SVD-decompose the data and estimate the covariance:

$$\mathbf{\Sigma} = \frac{1}{n-1}(\mathbf{USV}^T)^T(\mathbf{USV}^T) = \frac{1}{n-1}\mathbf{VSU}^T\mathbf{USV}^T$$

# Singular-Value Decomposition, SVD

## *Relation with Eigenvalue Decomposition*

Data  $\mathbf{X}$  (is now our  $\mathbf{A}$ ),      Data Covariance  $\mathbf{\Sigma} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$   
 $\mathbf{X} = \mathbf{USV}^T$

Let's SVD-decompose the data and estimate the covariance:

$$\mathbf{\Sigma} = \frac{1}{n-1}(\mathbf{USV}^T)^T(\mathbf{USV}^T) = \frac{1}{n-1}\mathbf{VSU}^T\mathbf{USV}^T = \mathbf{V}\frac{\mathbf{S}^2}{n-1}\mathbf{V}^T$$

# Singular-Value Decomposition, SVD

## *Relation with Eigenvalue Decomposition*

Data  $\mathbf{X}$  (is now our  $\mathbf{A}$ ),      Data Covariance  $\mathbf{\Sigma} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$   
 $\mathbf{X} = \mathbf{USV}^T$

Let's SVD-decompose the data and estimate the covariance:

$$\mathbf{\Sigma} = \frac{1}{n-1}(\mathbf{USV}^T)^T(\mathbf{USV}^T) = \frac{1}{n-1}\mathbf{VSU}^T\mathbf{USV}^T = \mathbf{V}\frac{\mathbf{S}^2}{n-1}\mathbf{V}^T$$

On the other hand,  $\mathbf{\Sigma}$  is symmetric, so can be diagonalised:

$$\mathbf{\Sigma} = \mathbf{VLV}^T$$

# Singular-Value Decomposition, SVD

## *Relation with Eigenvalue Decomposition*

Let's SVD-decompose the data and estimate the covariance:

$$\mathbf{\Sigma} = \frac{1}{n-1}(\mathbf{USV}^T)^T(\mathbf{USV}^T) = \frac{1}{n-1}\mathbf{VSU}^T\mathbf{USV}^T = \mathbf{V}\frac{\mathbf{S}^2}{n-1}\mathbf{V}^T$$

On the other hand,  $\mathbf{\Sigma}$  is symmetric, so can be diagonalised:

$$\mathbf{\Sigma} = \mathbf{VLV}^T$$

# Singular-Value Decomposition, SVD

## *Relation with Eigenvalue Decomposition*

Let's SVD-decompose the data and estimate the covariance:

$$\Sigma = \frac{1}{n-1}(\mathbf{USV}^T)^T(\mathbf{USV}^T) = \frac{1}{n-1}\mathbf{VSU}^T\mathbf{USV}^T = \mathbf{V}\frac{\mathbf{S}^2}{n-1}\mathbf{V}^T$$

On the other hand,  $\Sigma$  is symmetric, so can be diagonalised:

$$\Sigma = \mathbf{VLV}^T$$

- $\mathbf{L} = \frac{\mathbf{S}^2}{n-1}$ , eigenvalues  $\propto$  singular values
- $\mathbf{XV} = \mathbf{US}$ , principal components ( $\mathbf{XV}$ )  $\propto$  left singular vectors

# Singular-Value Decomposition, SVD

*SVD: Learn & Practice*

<https://nlp.stanford.edu/IR-book/pdf/18lsi.pdf>

Christopher D. Manning, Prabhakar Raghavan, and Hinrich Schütze. 2008. **Introduction to Information Retrieval**. Cambridge University Press, New York, NY, USA.

# Comments & Final Remarks

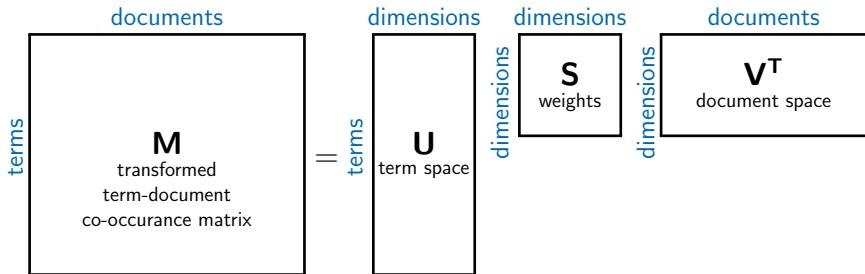
## *Outline*

- 1 Introduction
- 2 Principal Component Analysis, PCA
- 3 Singular-Value Decomposition, SVD
- 4 Comments & Final Remarks
  - LSA
  - Limitations of PCA
  - LDA
  - t-SNE



# Comments & Final Remarks

## *SVD: Application, Latent Semantic Analysis (LSA/LSI)*



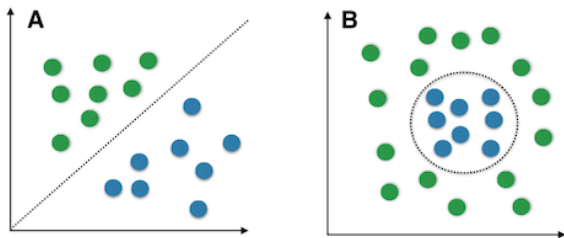
$$S_r \Rightarrow M_r$$

# Comments & Final Remarks

## *Limitations of PCA*

The useful projections **might not** be **linear**

Linear vs. nonlinear problems

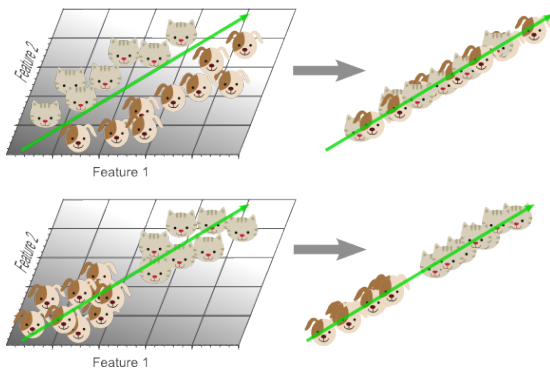


[https://sebastianraschka.com/Articles/2014\\_kernel\\_pca.html](https://sebastianraschka.com/Articles/2014_kernel_pca.html)

# Comments & Final Remarks

## *Limitations of PCA*

The most discriminative information **might not** be captured by the largest **variance**

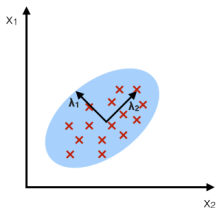


# Comments & Final Remarks

## *General PCA vs. Linear Discriminant Analysis (LDA)*

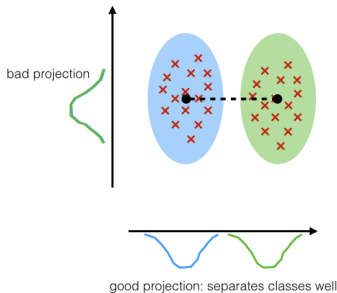
### **PCA:**

component axes that maximize the variance



### **LDA:**

maximizing the component axes for class-separation



[https://sebastianraschka.com/Articles/2014\\_python\\_lda.html](https://sebastianraschka.com/Articles/2014_python_lda.html)

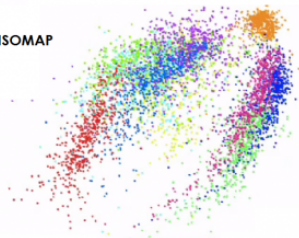
# Comments & Final Remarks

## *Visualisation: t-SNE*

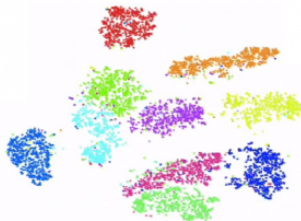
PCA



ISOMAP



T-SNE



# Comments & Final Remarks

*Visualisation: t-SNE*

## **t-Distributed Stochastic Neighbor Embedding**

- Completely different approach to PCA
- Non-linear technique

# Comments & Final Remarks

*Visualisation: t-SNE*

## t-Distributed Stochastic Neighbor Embedding

- Completely different approach to PCA
- Non-linear technique

### Description

- Probability of similarity of points in high-D space
- Probability of similarity of points in low-D space
- Minimise the difference between these conditional probabilities in high-D and low-D spaces

# Comments & Final Remarks

## Comments on Visualisation

believe	0.193
consider	0.416
thinks	0.432
thought	0.432
feel	0.443
believes	0.492
thinking	0.522
know	0.531
pense	0.539
believed	0.549





Thanks!

Questions?

# PCA, SVD and Other Related Acronyms

**Cristina España-Bonet**

UdS & DFKI, Saarbrücken, Germany

Summer Semester Seminar

15th May 2019