A Brief Introduction to Principal Component Analysis

Immeidately followed by a longer introduction...

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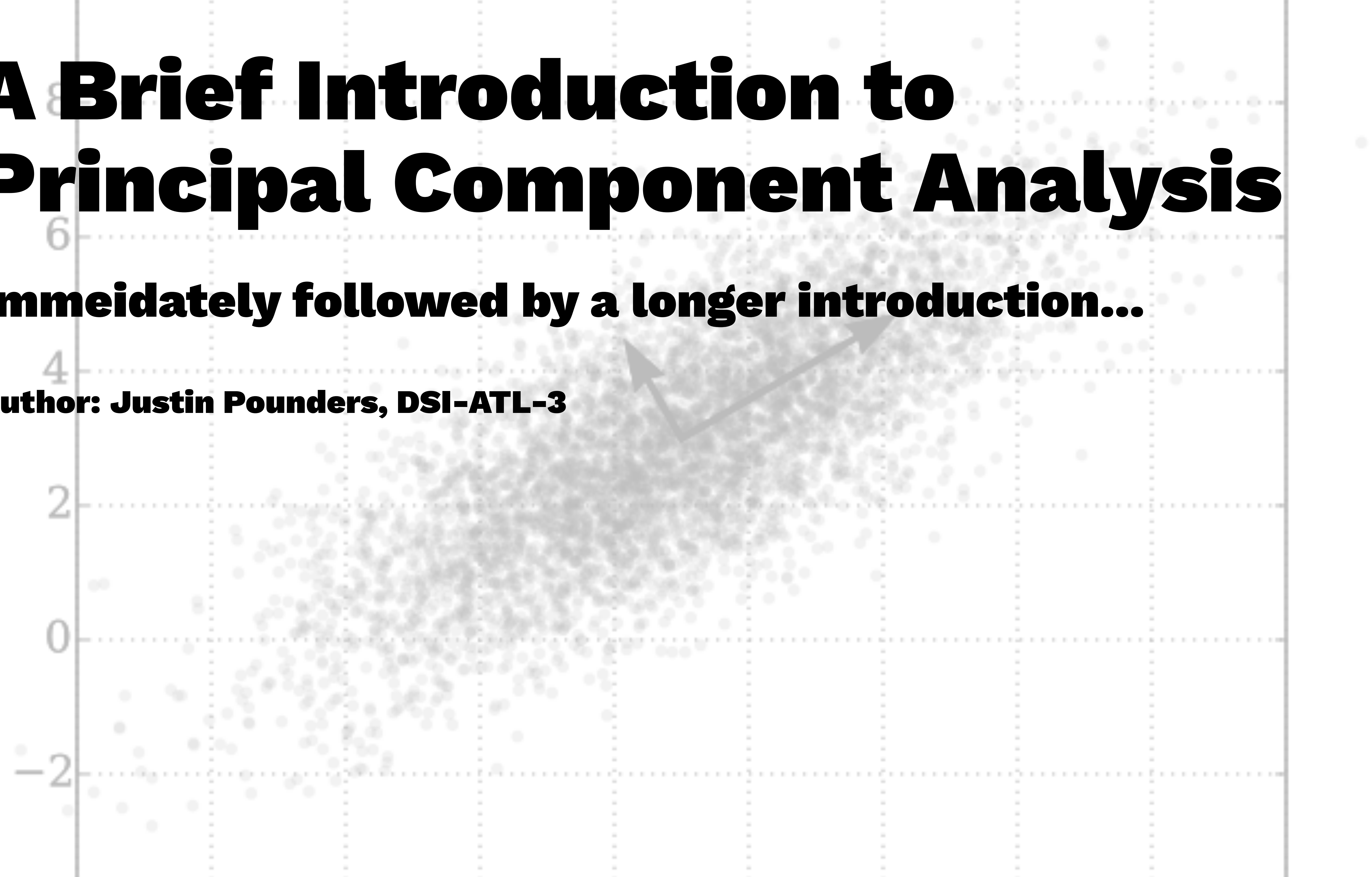


PCA = Principle Component Analysis

Goals:

- Transform original variable/features into new, "high-performance" features
- Reduce the dimensionality of the data
- Eliminate multicollinearity

Intro to PCA

Say that I want to predict **age** from stress, income and health.

1. Three-dimensional data
2. Multicollinearity probably exists

PCA will give me one or two **super-predictor** variables called components (hopefully).

Intro to PCA

Principal components:

$$PC1 = w_{1,1}(\text{stress}) + w_{2,1}(\text{income}) + w_{3,1}(\text{health})$$

$$PC2 = w_{1,2}(\text{stress}) + w_{2,2}(\text{income}) + w_{3,2}(\text{health})$$

$$PC3 = w_{1,3}(\text{stress}) + w_{2,3}(\text{income}) + w_{3,3}(\text{health})$$

Intro to PCA

This is cool because...

- $PC1$ is better than $PC2$ is better than $PC3$
- All of these are uncorrelated

Now for the slightly longer version...

Motivation

— Dimensionality reduction reduces the number of random variables that you are considering for analysis

— To get a quick summary of our data, we can calculate a covariance matrix, an unstandardized correlation matrix.

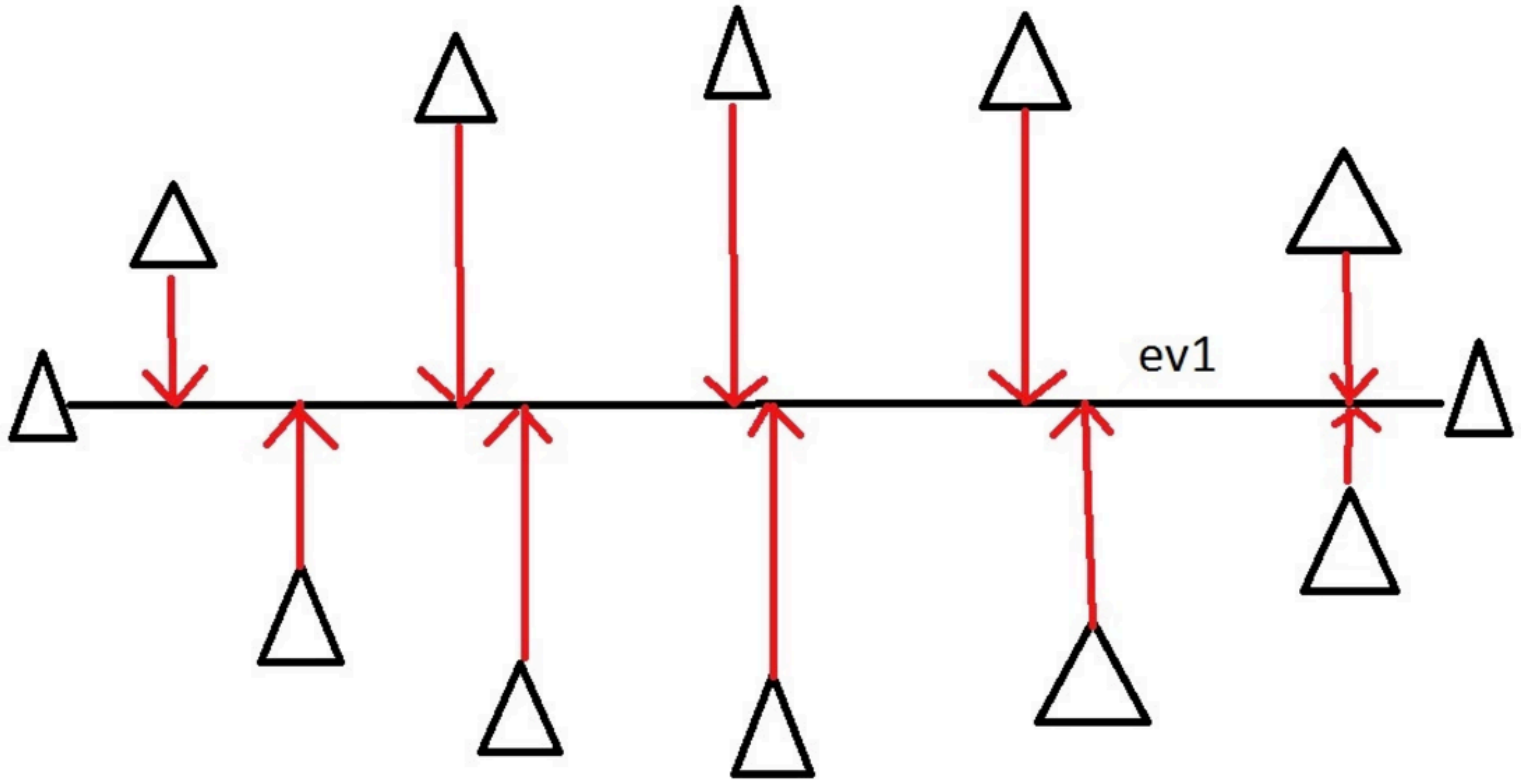
Motivation

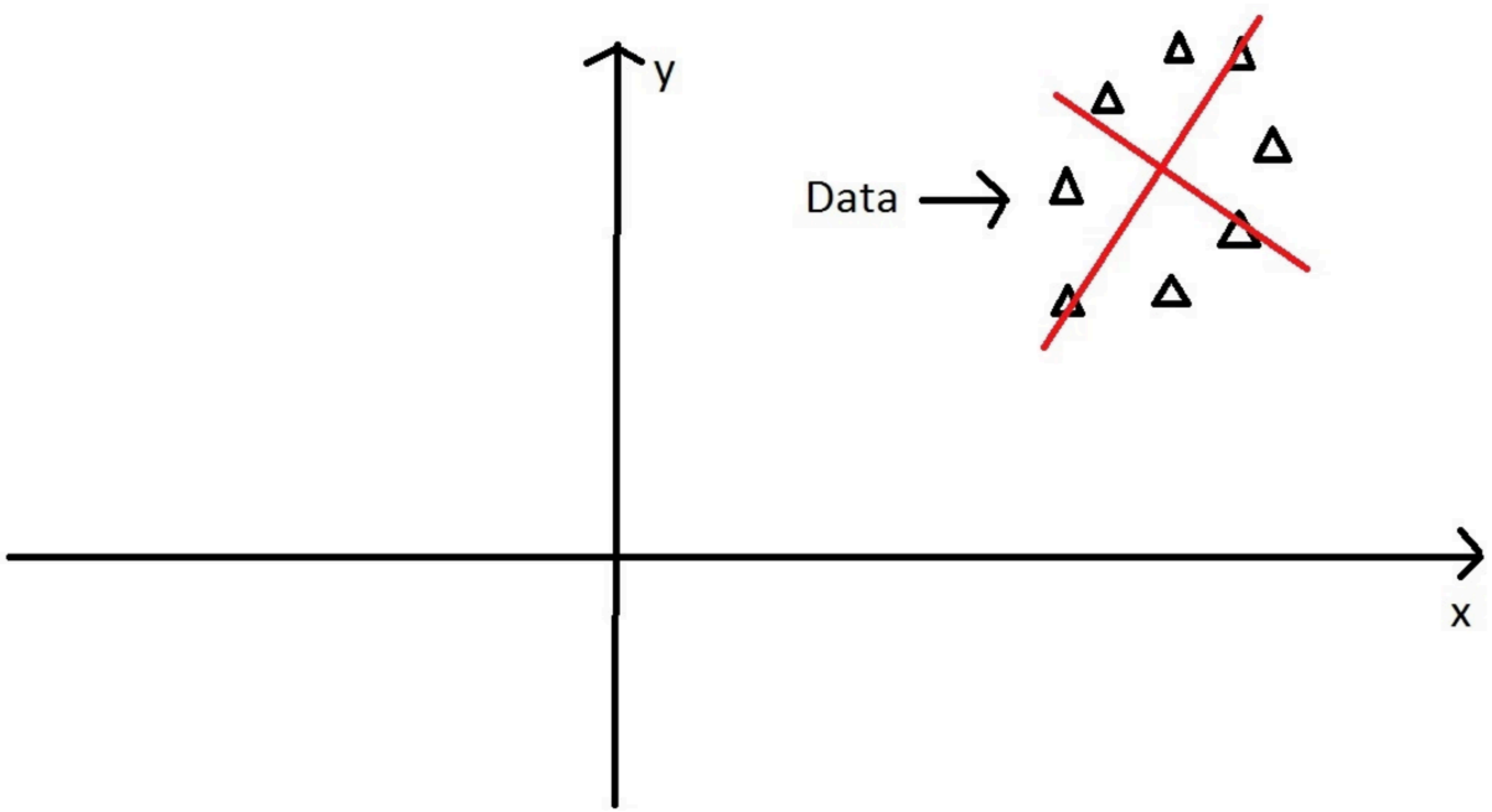
What would an 'ideal' covariance matrix look like?
- Large numbers on diagonal
- Small numbers off diagonal

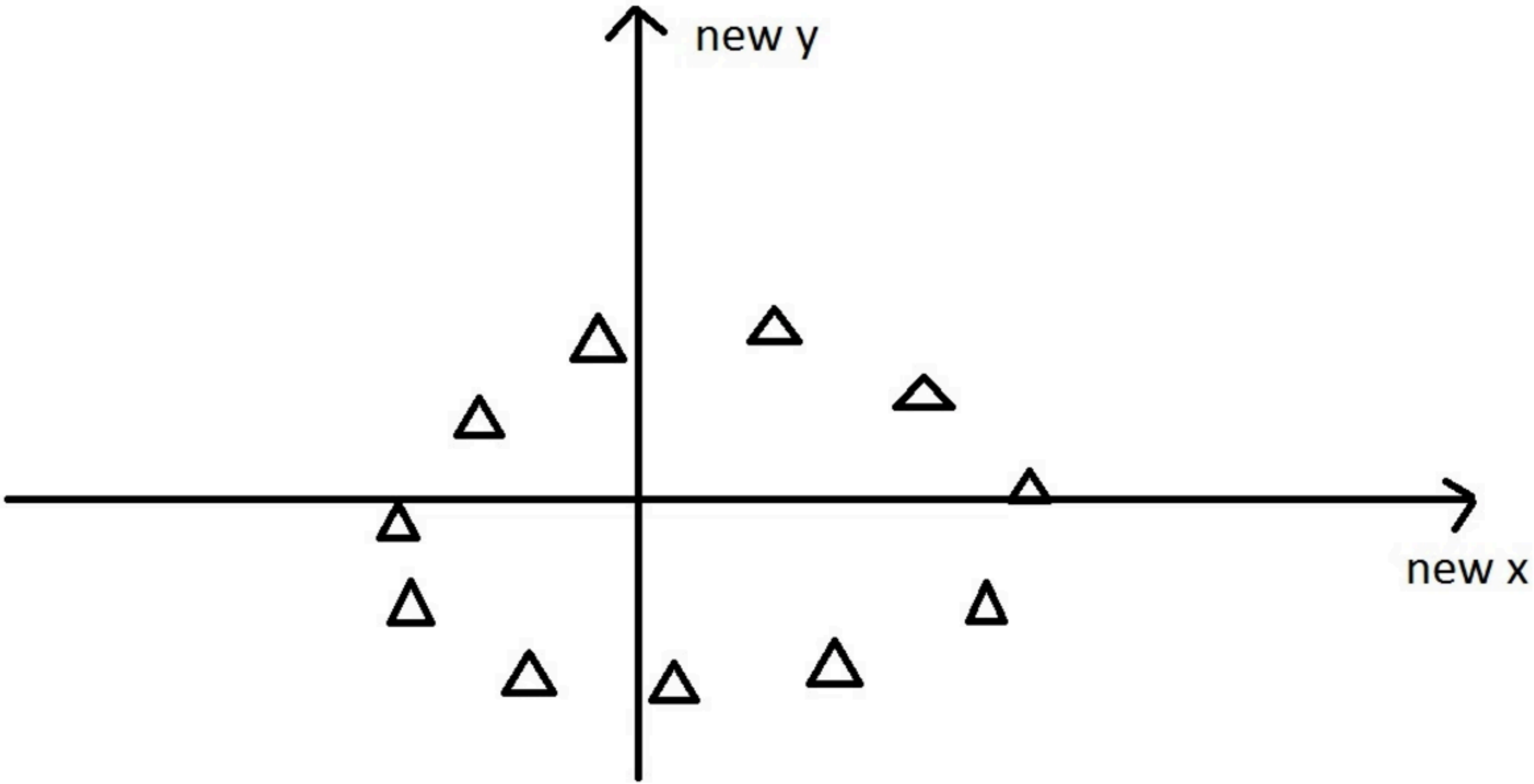
Principal Component Analysis

- PCA finds linear combinations of current predictor variables that...
- create new "principal components". The principal components explain...
- the maximum possible amount of variance in your predictors.

Think of PCA as a coordinate transformation. The old axes are the original variables (columns). The new axes are the principal components from PCA.


ev1


y
Data
x


new y
new x

PCA is nothing but coordinate system transformation: A simple example

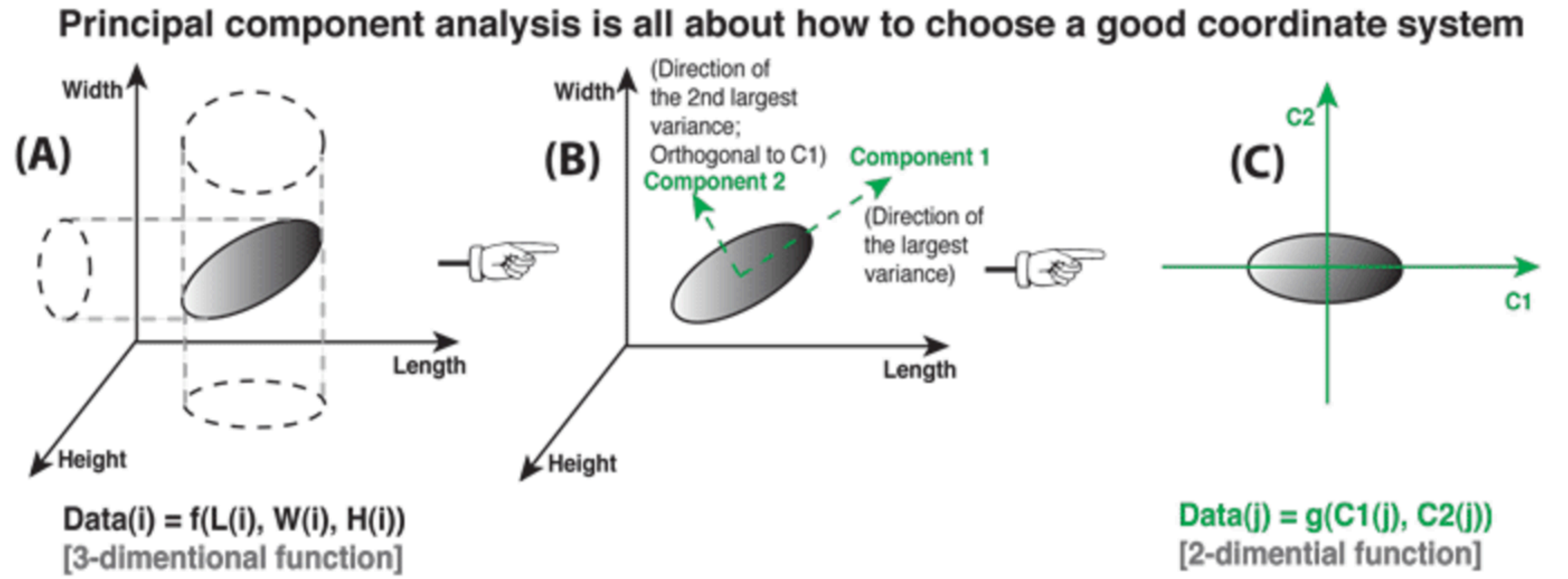


Figure 1. (A) A simple object described by a complex set of variables (or coordinate system). (B) Find new variables (coordinate axes) orthogonal to each other and pointing to the direction of largest variances. (C) Use new variables (coordinate axes) to describe object in a more concise way.

Mathematical Details

- We are looking for new directions in feature space
- Each consecutive direction tries to maximize remaining variance
- Each direction is orthogonal to all the others

What does that mean?

The inputs `stress`, `income` and `health`...

...can be replaced with 3 new variables...

— PC1 $\rightarrow$ most variance

— PC2

— PC3 $\rightarrow$ least variance (noise?)

Principal components

$$PC1 = w_{1,1}(\text{stress}) + w_{2,1}(\text{income}) + w_{3,1}(\text{health})$$

$$PC2 = w_{1,2}(\text{stress}) + w_{2,2}(\text{income}) + w_{3,2}(\text{health})$$

$$PC3 = w_{1,3}(\text{stress}) + w_{2,3}(\text{income}) + w_{3,3}(\text{health})$$

Explaining PCA

The weights are called loadings

— They are coefficients indicating how heavily each of the input data are weighted

e.g.

$$PC1 = 0.01(\mathbf{stress}) - 0.54(\mathbf{income}) + 0.71(\mathbf{health})$$

We will see how to get these values from `sklearn`

Explaining PCA

The total variance of your data gets redistributed among the principal components:

$$\mathrm{var}(PC1) > \mathrm{var}(PC2) > \mathrm{var}(PC3)$$

Interpreting PCA: Signal v. Noise

PCA attempts to maximize signal (high variance) while isolating noise (low variance)

- Most variance captured in first several principal components
- Noise isolated to last several principal compoments
- This done simultaneously across all input variables

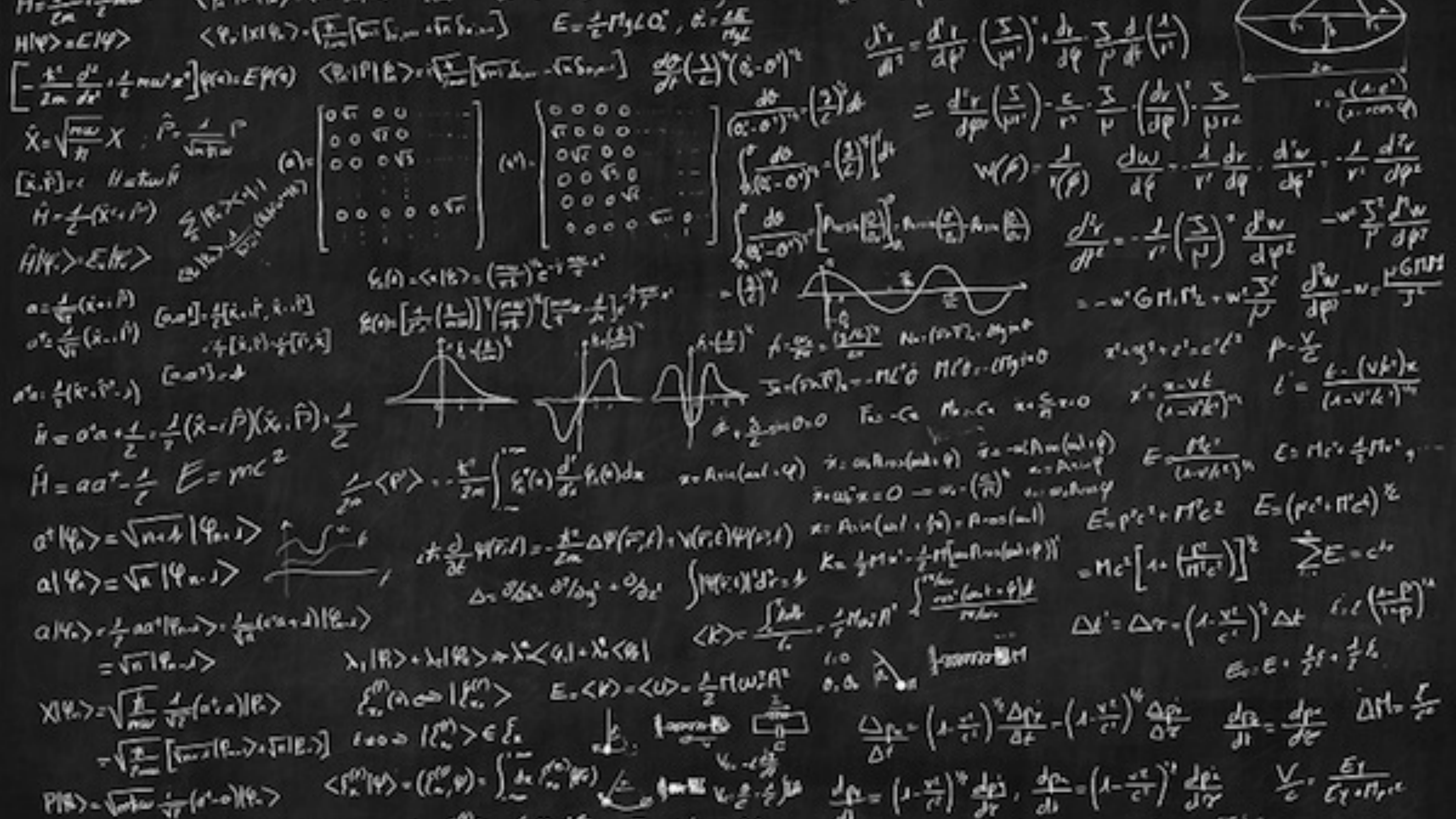
Explaining PCA

There is no covariance between principal components

$$\mathrm{covar}(PC1, PC2) = 0$$

$$\mathrm{covar}(PC1, PC3) = 0$$

$$\mathrm{covar}(PC2, PC3) = 0$$


$E = mc^2$

The Math Foundation

Eigenvalue decomposition of covariance matrix
This diagonalizes the covariance matrix.

The principal component transformation
This transforms each input variable onto a new orthogonal basis in which the new variables are maximally variant.

$$\mathbf{Z} = \mathbf{X}\mathbf{W}$$

Introduction to Statistical Lerning section 10.2 has a great overview that is of medium technical complexity.

Summary

1. What is the output of PCA?
2. Why is PCA useful?

Turn and talk.

Python Time

Go to `intro-to-PCA.ipynb`.