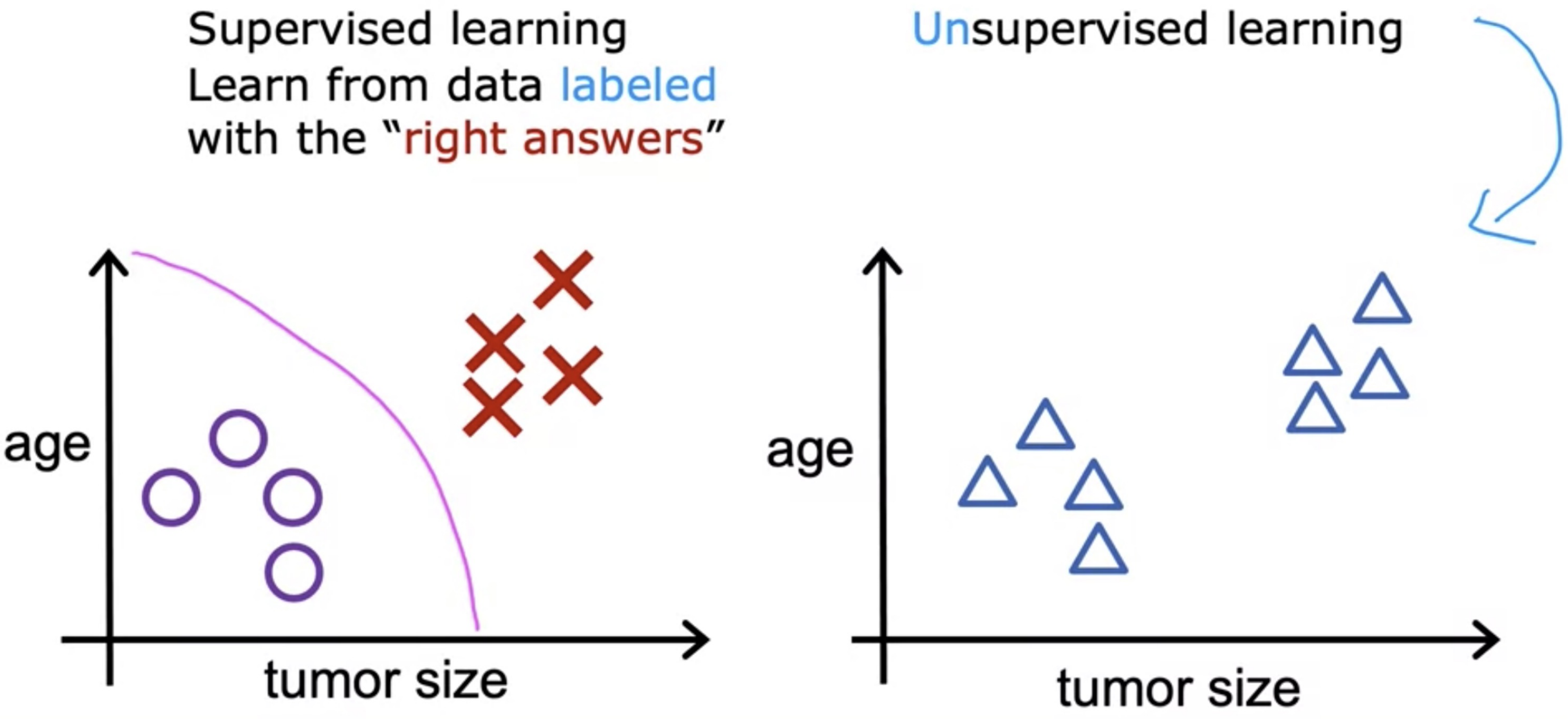
AIBridge

Lecture 8

Introducing Unsupervised Learning



Credit: Andrew Ng, [Machine Learning]

Unsupervised Learning

Clustering
Dimension reduction

Clustering: Google news

Giant panda gives birth to rare twin cubs at Japan's oldest zoo

USA TODAY · 6 hours ago

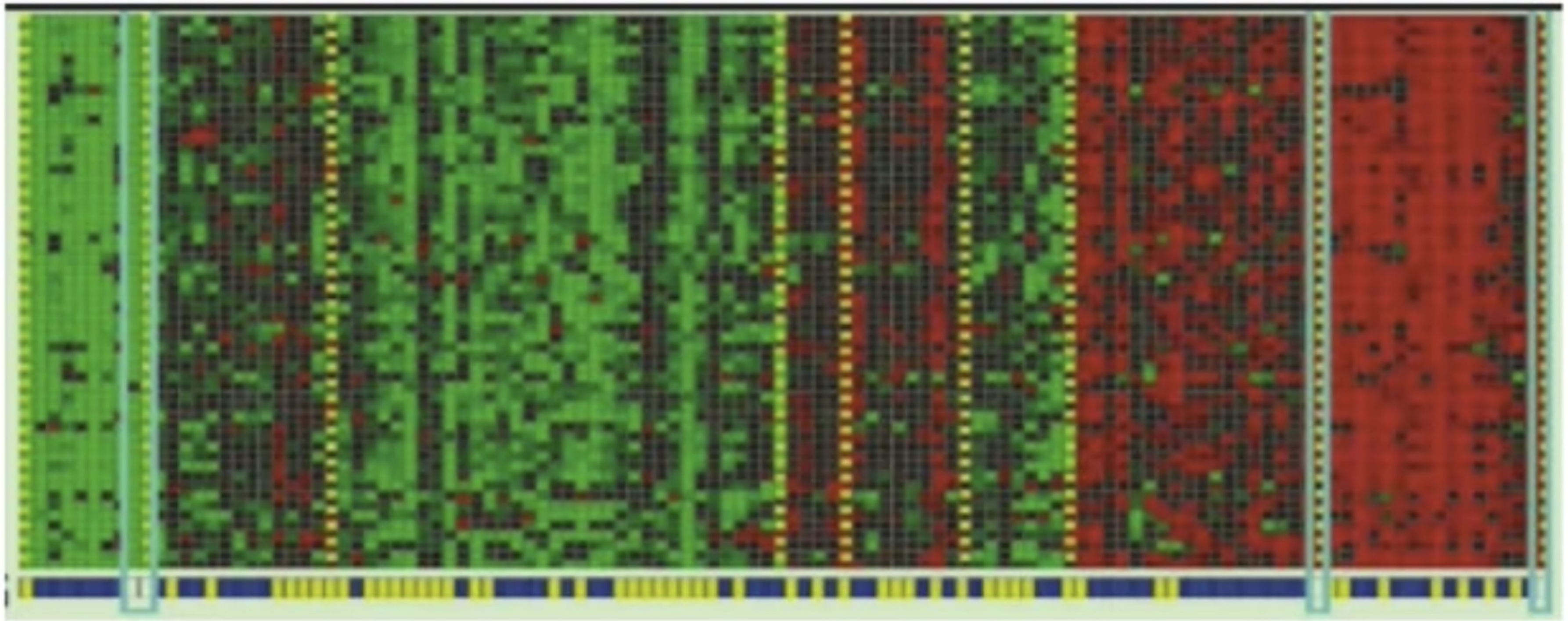
- **Giant panda gives birth to twin cubs at Japan's oldest zoo**
  CBS News · 7 hours ago
- **Giant panda gives birth to twin cubs at Tokyo's Ueno Zoo**
  WHBL News · 16 hours ago
- **A Joyful Surprise at Japan's Oldest Zoo: The Birth of Twin Pandas**
  The New York Times · 1 hour ago
- **Twin Panda Cubs Born at Tokyo's Ueno Zoo**
  PEOPLE · 6 hours ago

View Full Coverage

Credit: Andrew Ng, Machine Learning

Clustering: DNA microarray

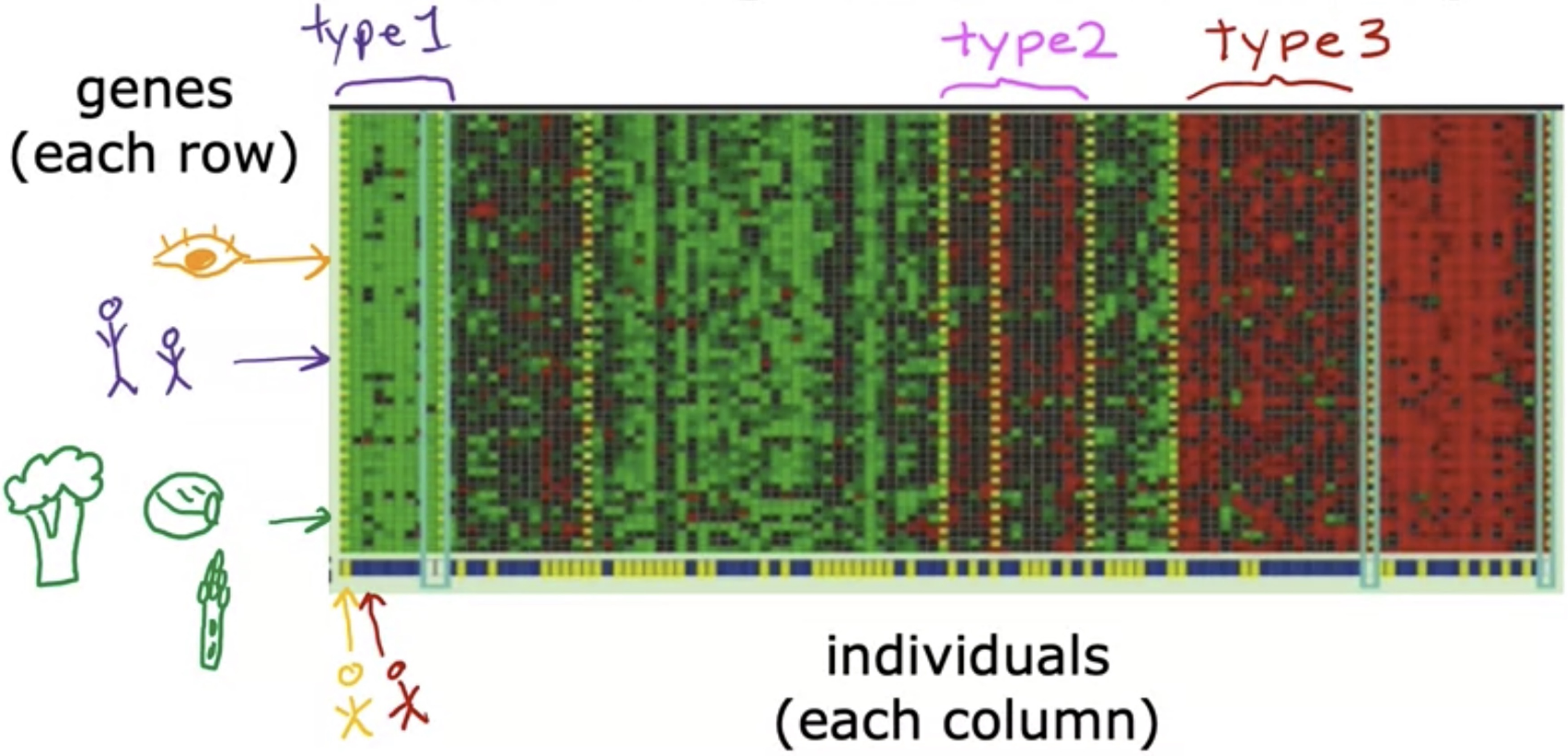
genes
(each row)



individuals
(each column)

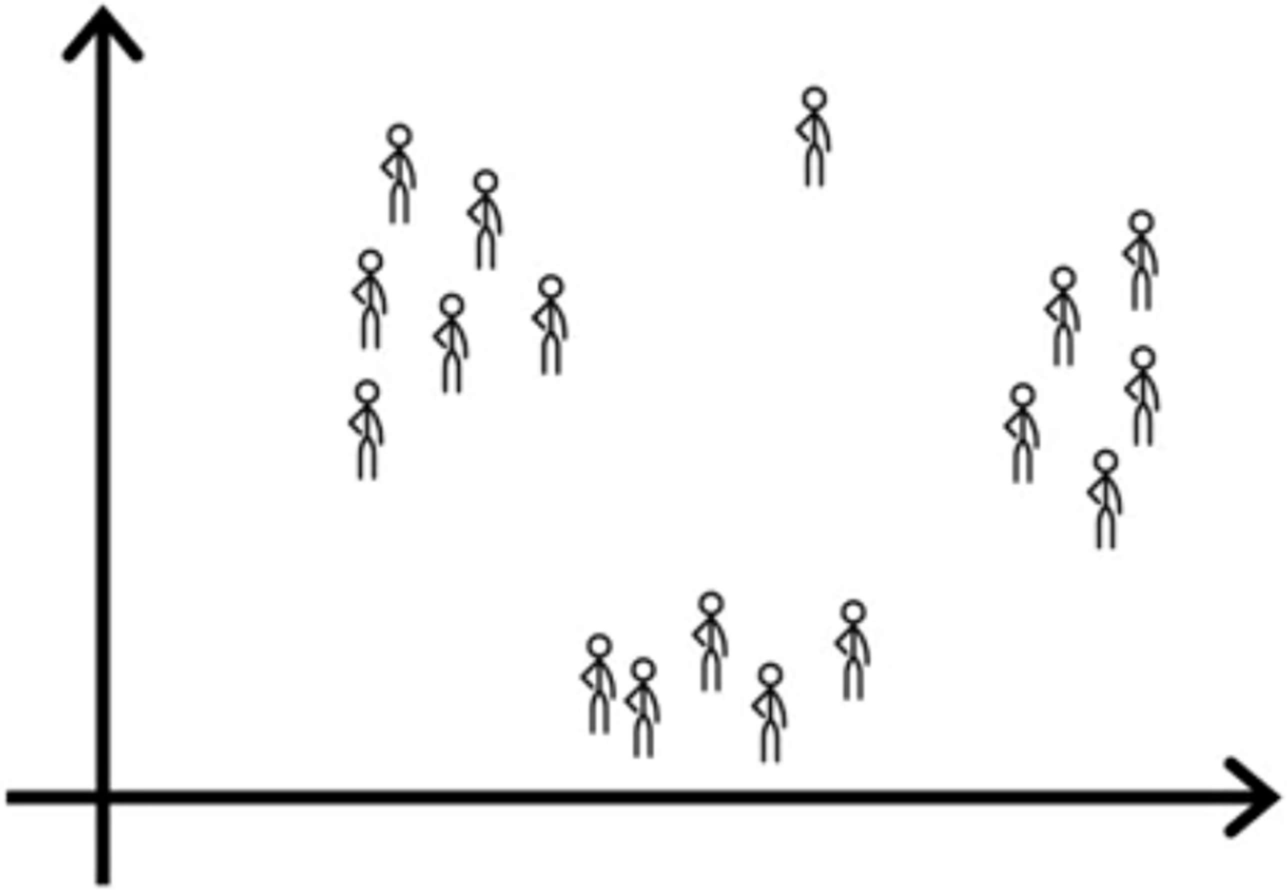
Credit: Andrew Ng, [Machine Learning]

Clustering: DNA microarray



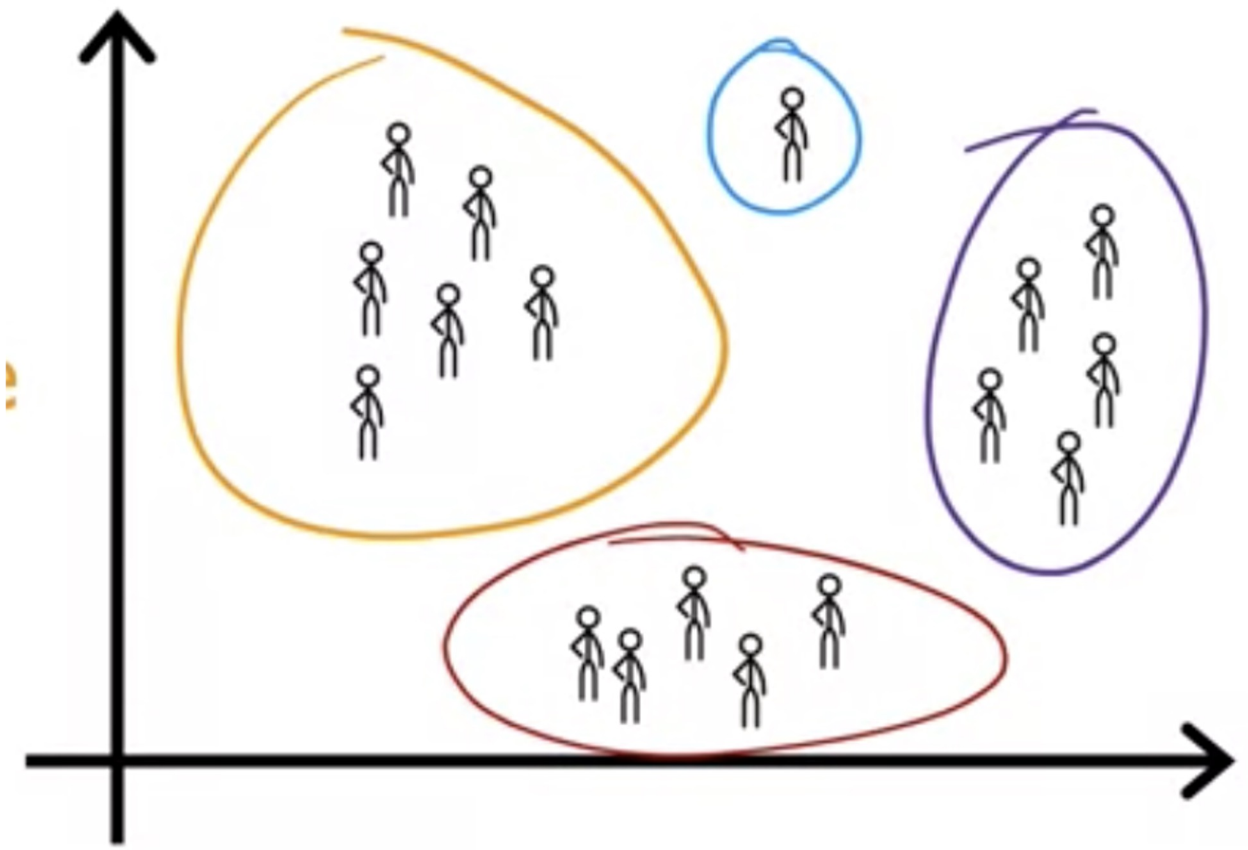
Credit: Andrew Ng, [Machine Learning]()

Clustering: Grouping customers



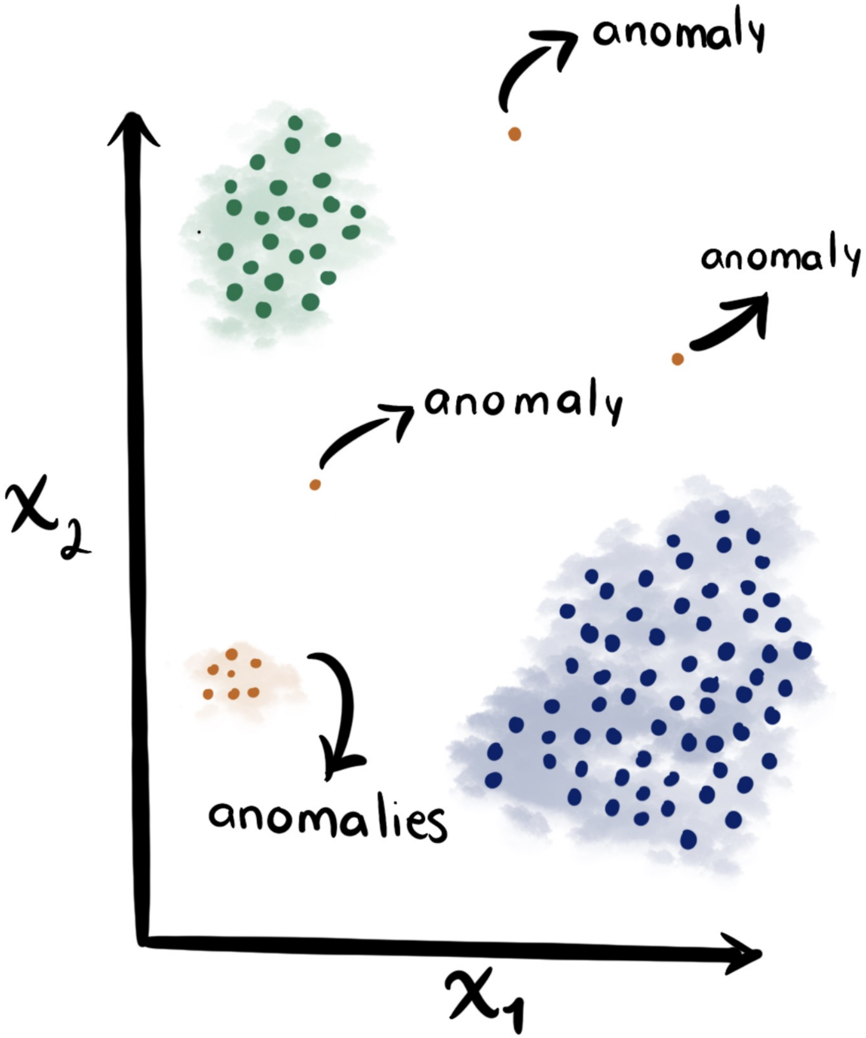
Credit: Andrew Ng, Machine Learning

Grouping Customers



Credit: Andrew Ng, Machine Learning

Anomaly Detection



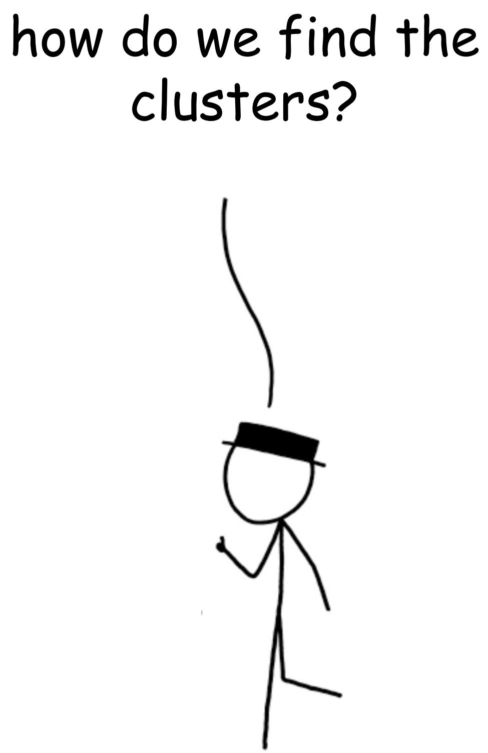
Credit: [Anomaly Detection]

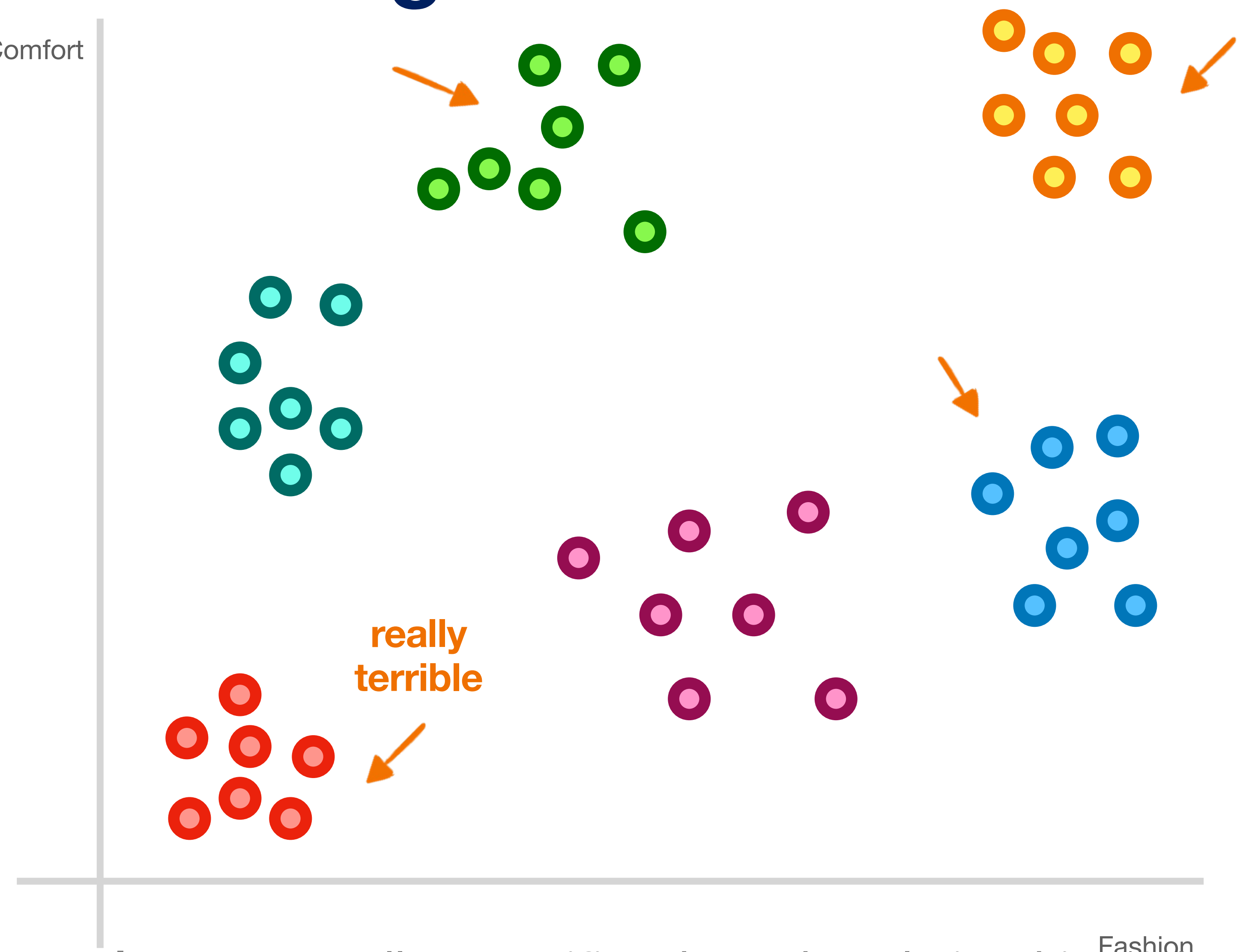
Unsupervised Learning

Clustering

Dimension reduction

K-means clustering

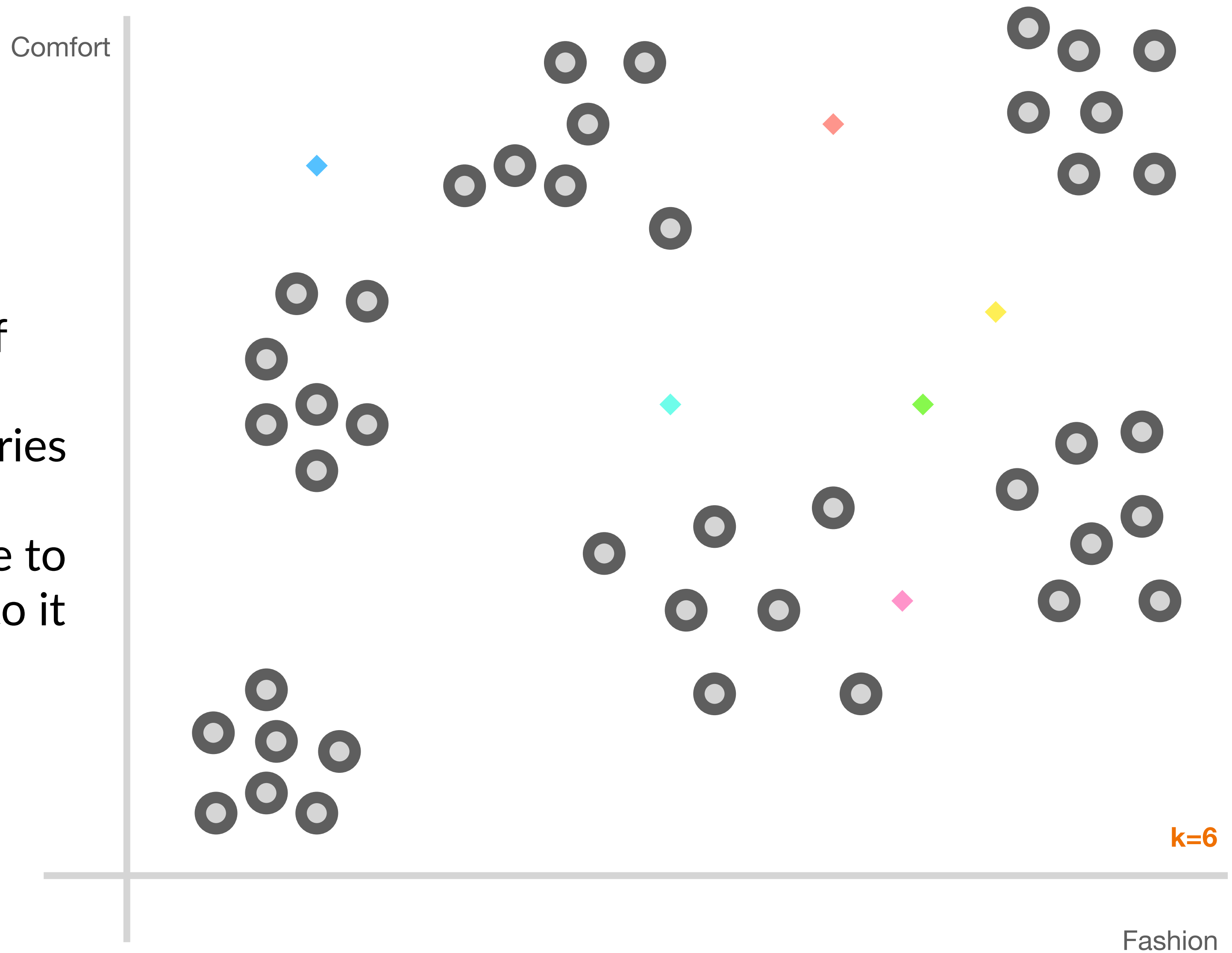




clusters can tell us specifics about the relationship of data

...even if they are unlabeled! → **unsupervised learning!**

1. pick a K-number of clusters
2. randomly pick a series of “**centroids**”
3. assign each particle to the **centroid** closest to it



1. pick a K-number of clusters
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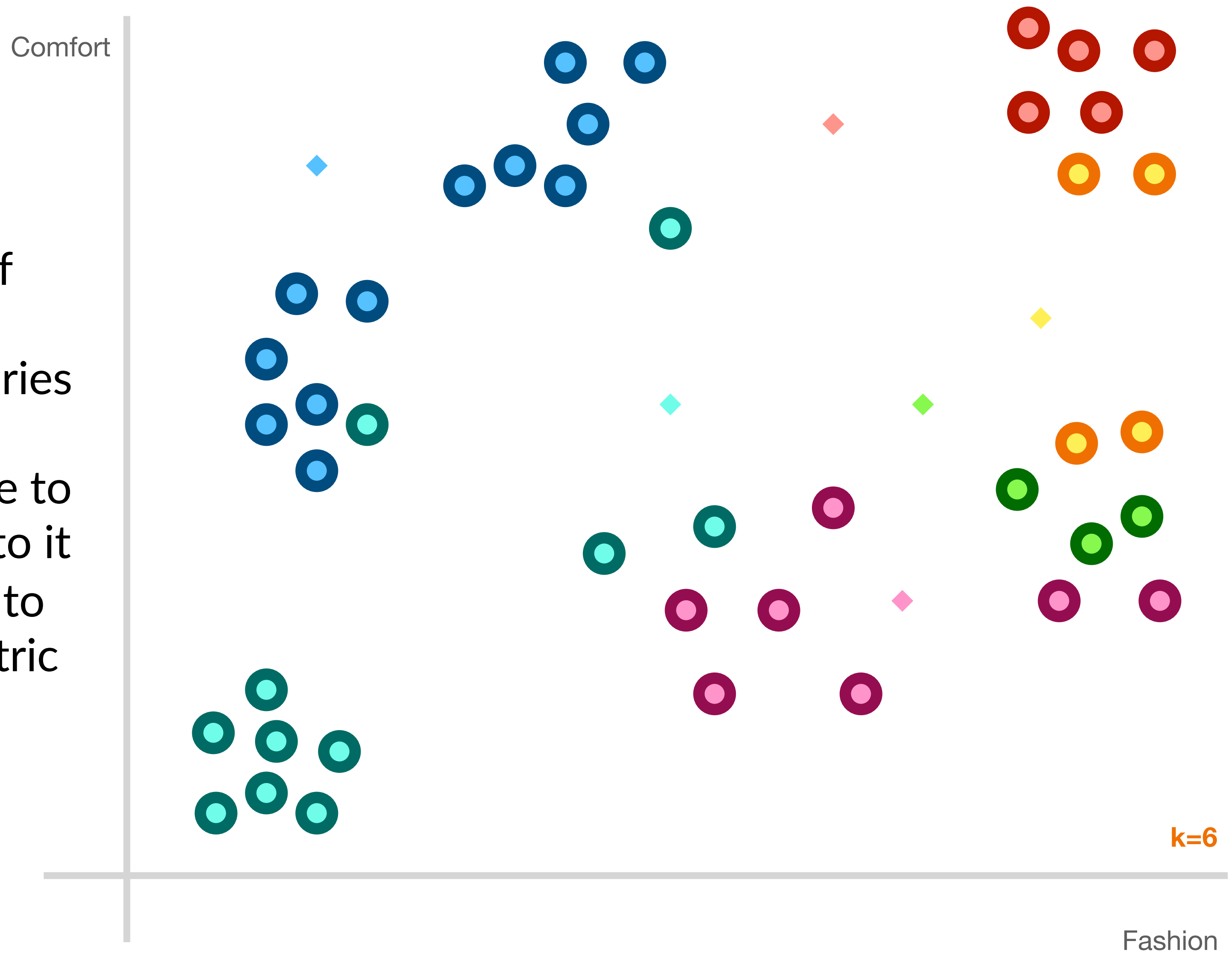
4. move the **centroid** to the weighted geometric center of samples assigned to it



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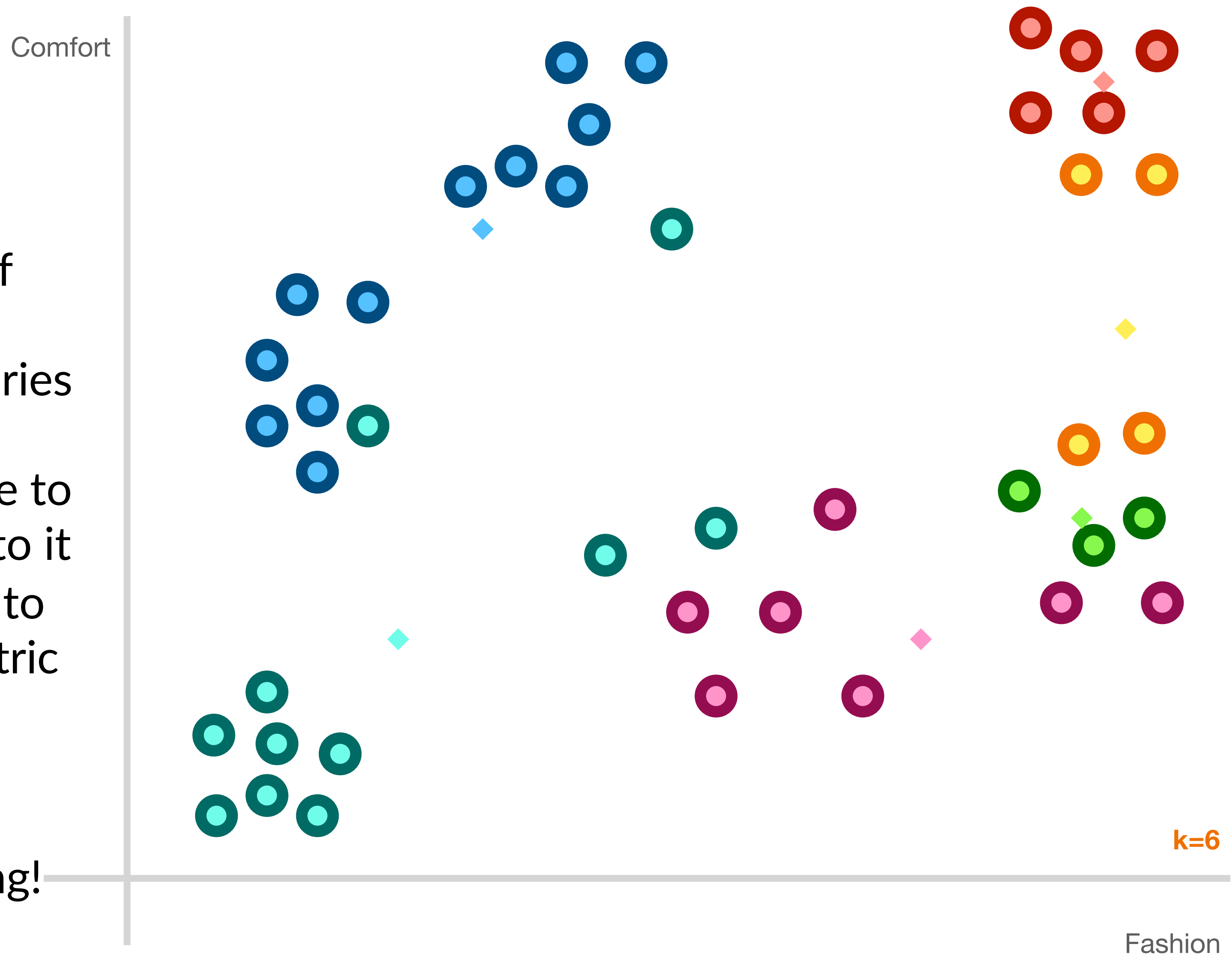
4. move the **centroid** to the weighted geometric center of samples assigned to it
5. Repeat 3-4 until centroids stop moving!



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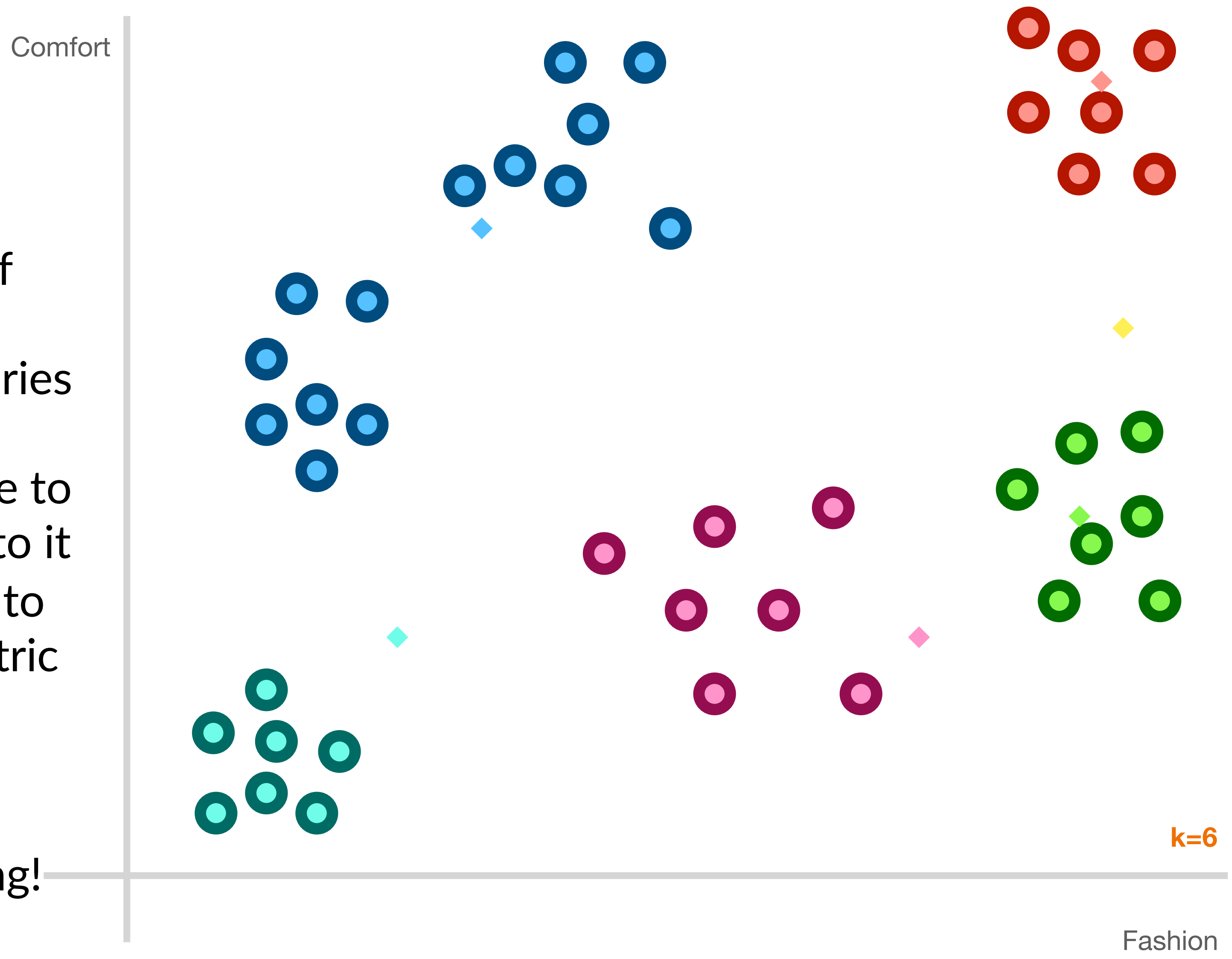

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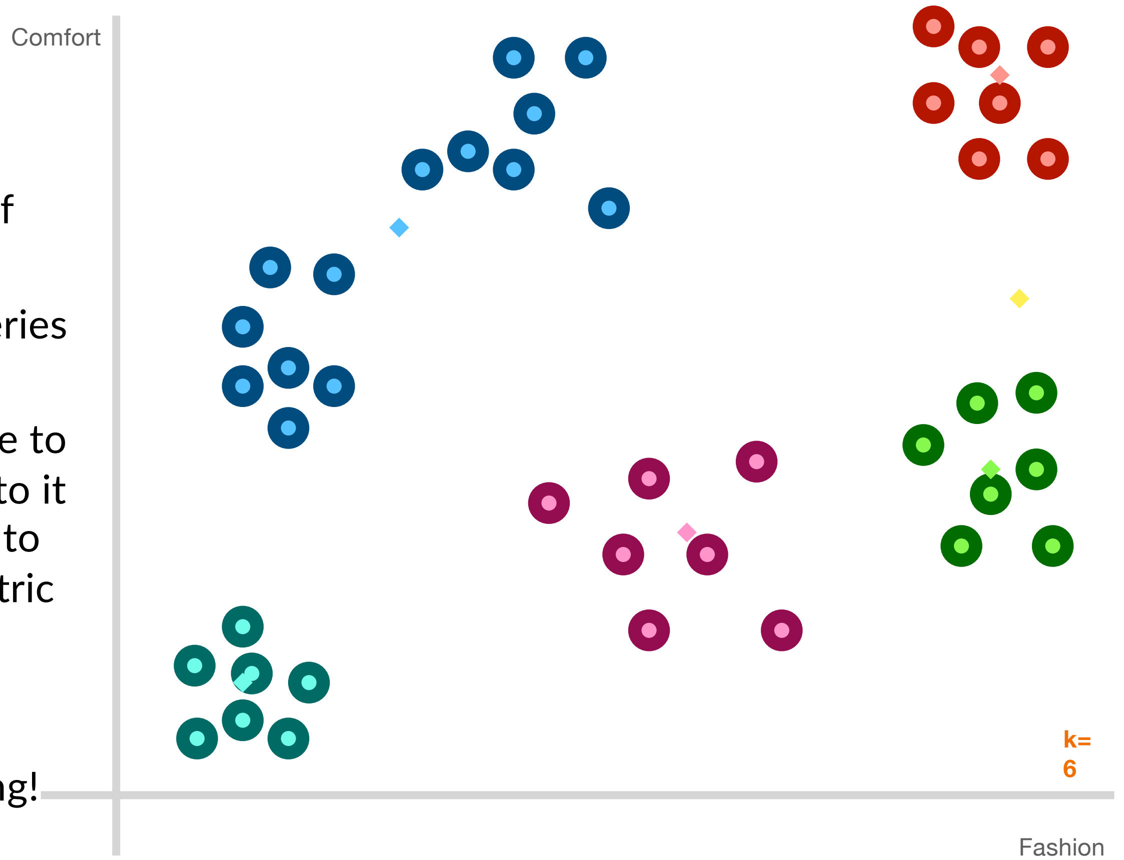


Did we get back the same clusters?

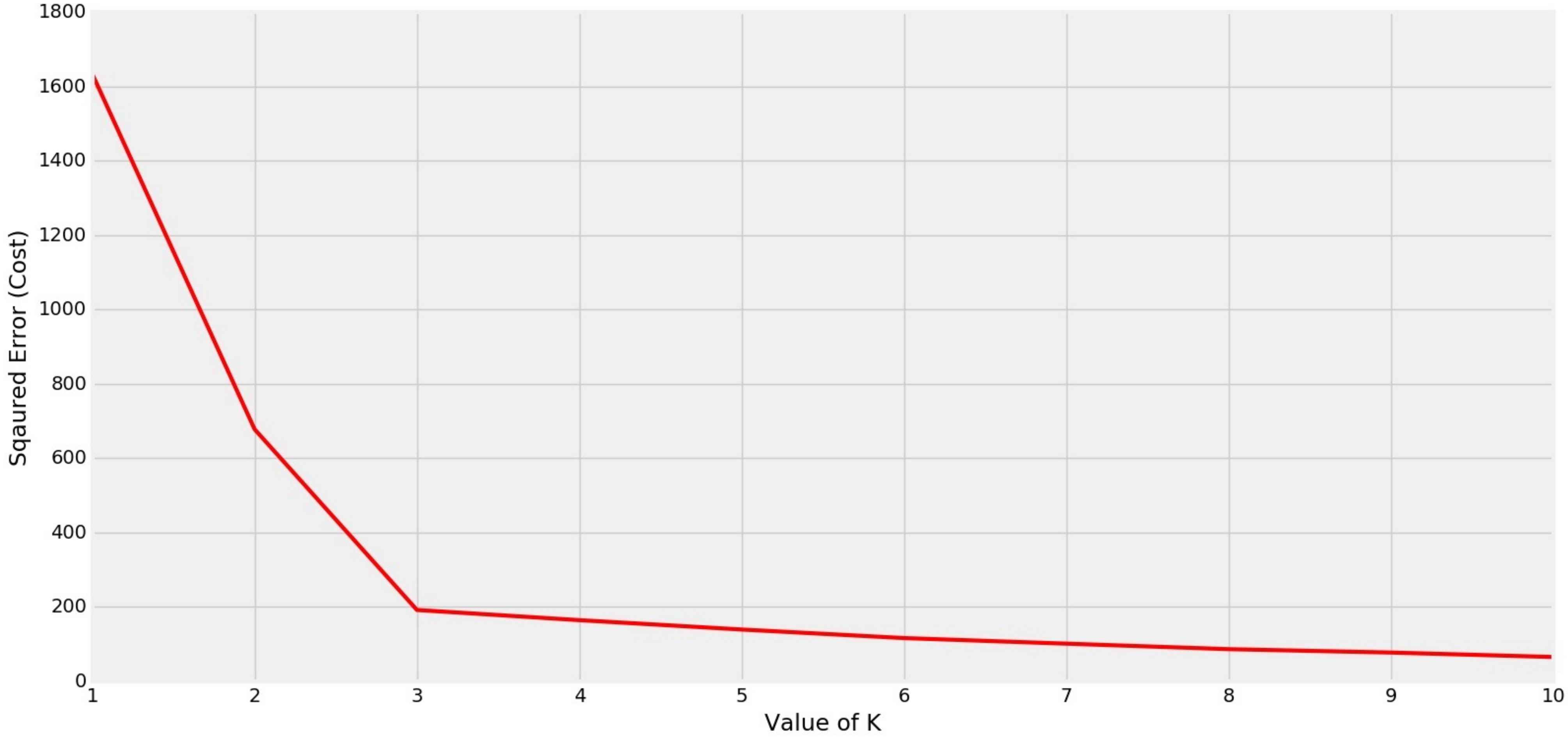
Nope. And that’s OK.

Did we get back the same clusters?

Nope. And that's OK.

K-means is an *indeterministic* algorithm—it has built-in randomness

Evaluation and Choosing K



Unsupervised Learning

Clustering

Dimension reduction

Unsupervised Learning

Why Dimension reduction?

Motivation for Dimension Reduction

Complex systems often must be modeled with large datasets, having dozens to millions of columns.

Often, several columns can be adding similar information to the model. So, there is a certain level of *redundancy.*

A

Individual	Height (cm)	Weight (kg)	Income ($)	Number of Children
Person A	165	65	60,000	2
Person B	168	63	100,000	5
Person C	159	82	50,000	1
Person D	183	68	90,000	4
Person E	187	87	110,000	5
Person F	189	89	95,000	4

Four dimensions; can't even be graphed!

Motivation for Dimension Reduction

Individual	Height (cm)	Weight (kg)	Income ($)	Number of Children
Person A	165	65	60,000	2
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What if I have a lot of features, but not a lot of samples?

Motivation for Dimension Reduction

Individual	Height (cm)	Weight (kg)	Income ($)	Number of Children
Person A	165	65	60,000	2
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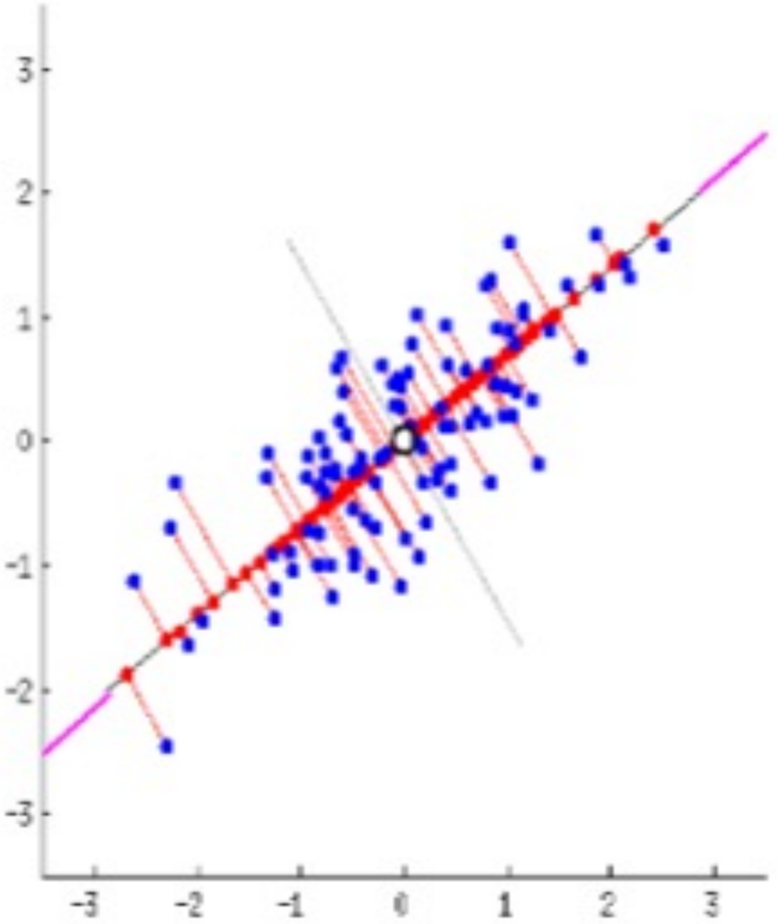
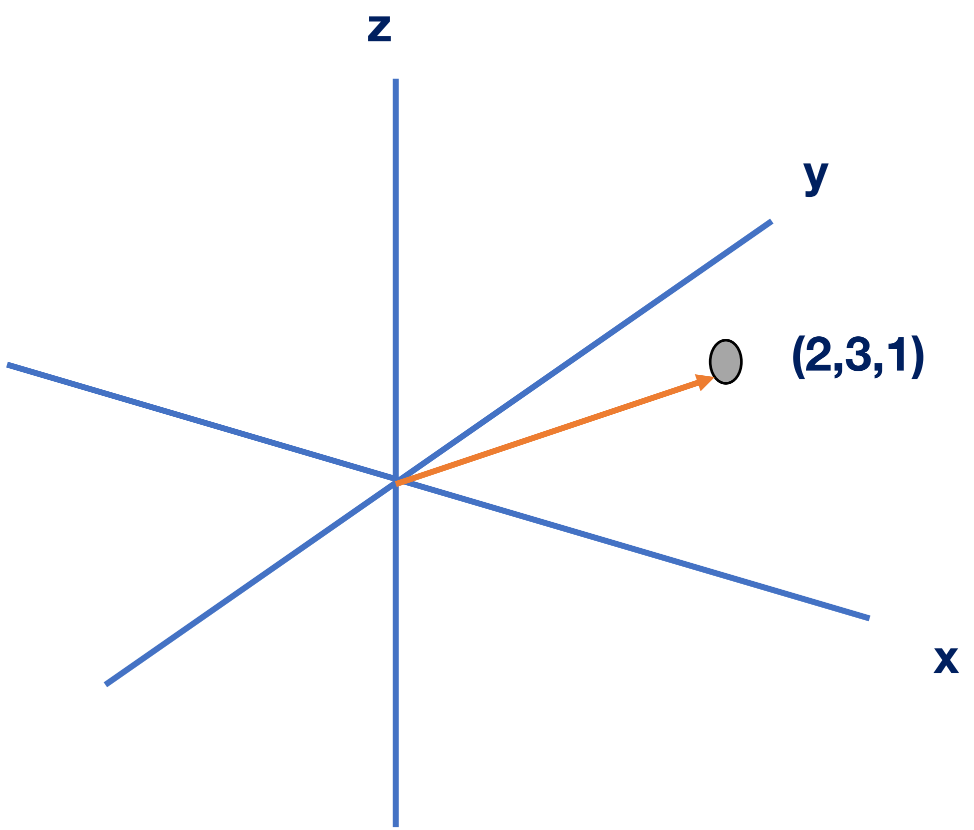
Enter…

Principal Component Analysis

Principle Component Analysis



Exploring Dimensions and Basis Vectors

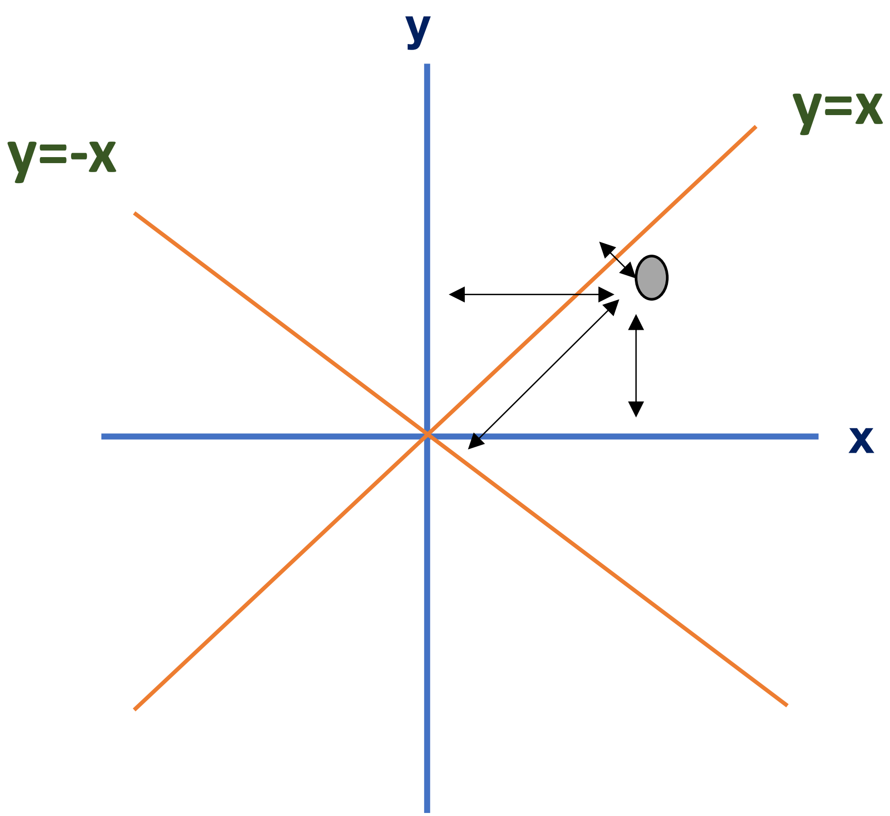


(2,3,1) is a datapoint.

$$\begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}$$ **is the vector to said datapoint.**

Dimension = # of features

Exploring Dimensions and Basis Vectors

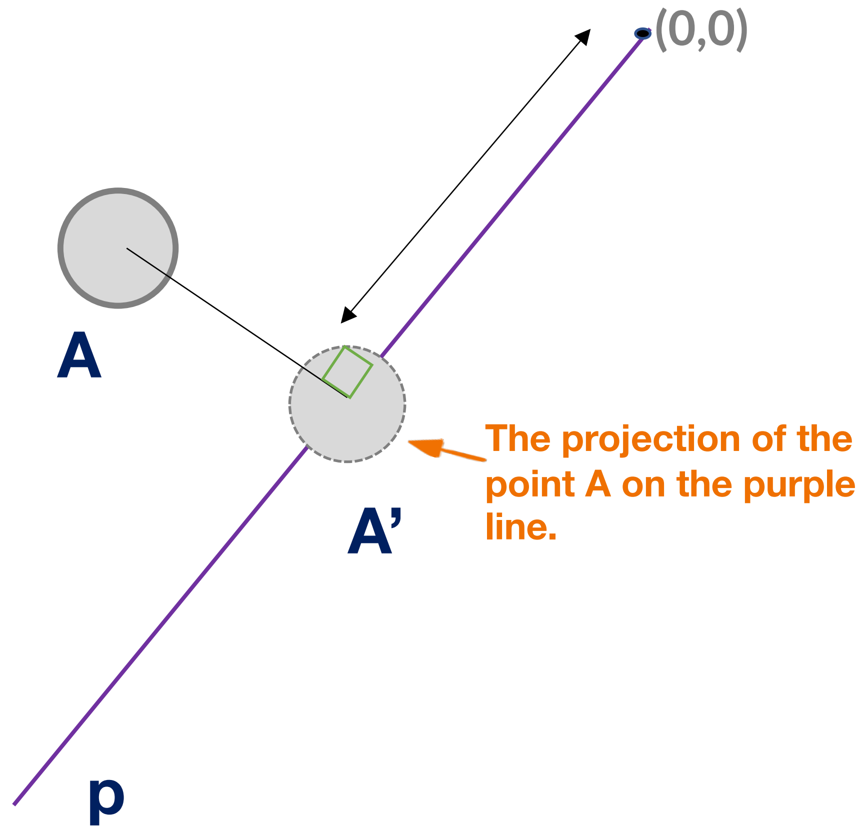


This gray point can be expressed as 3 blocks on x axis and 2 blocks on the y axis.

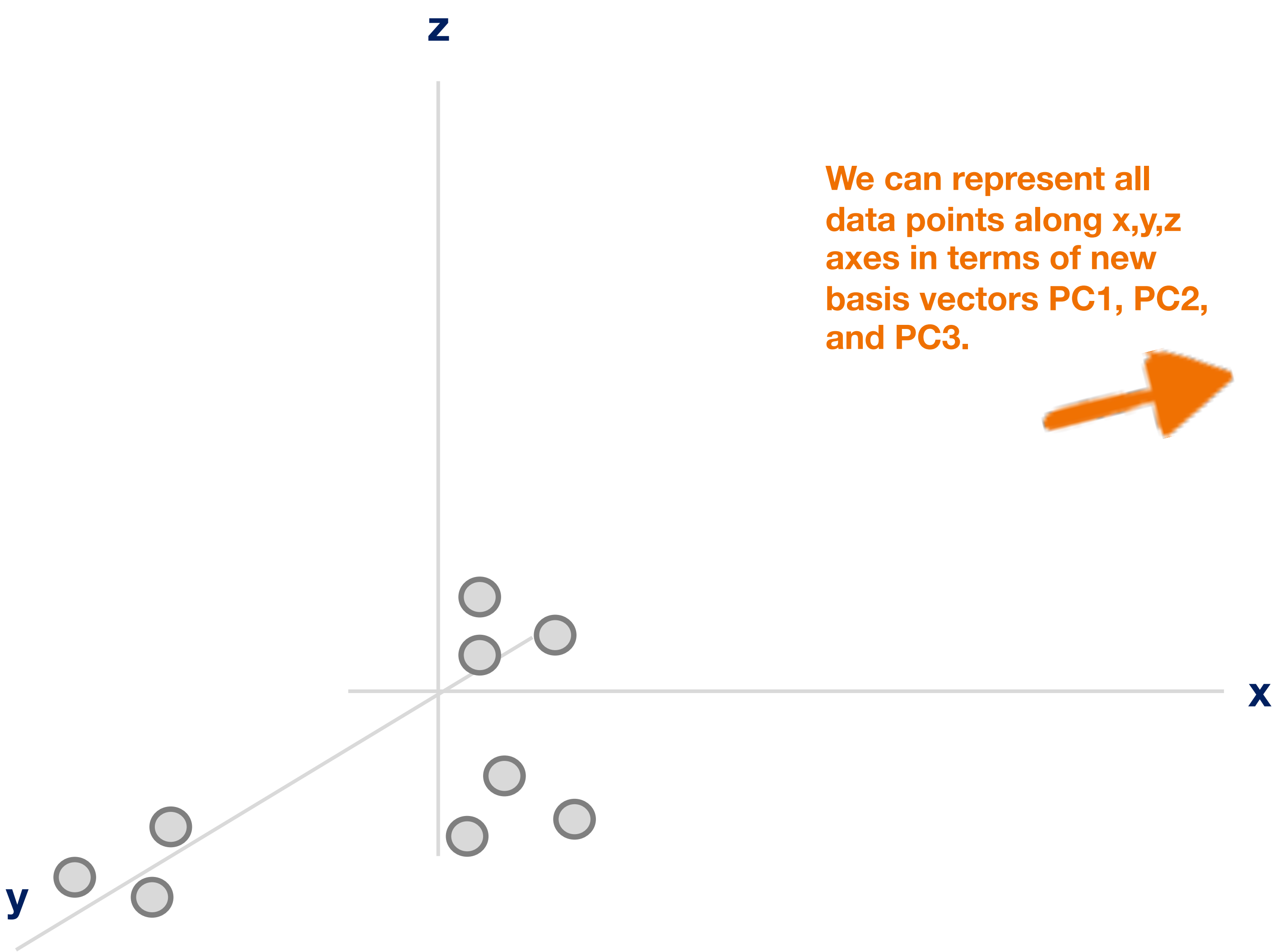
It can also be expressed as 1 block on y = -x and 3 blocks on y=x

Projection

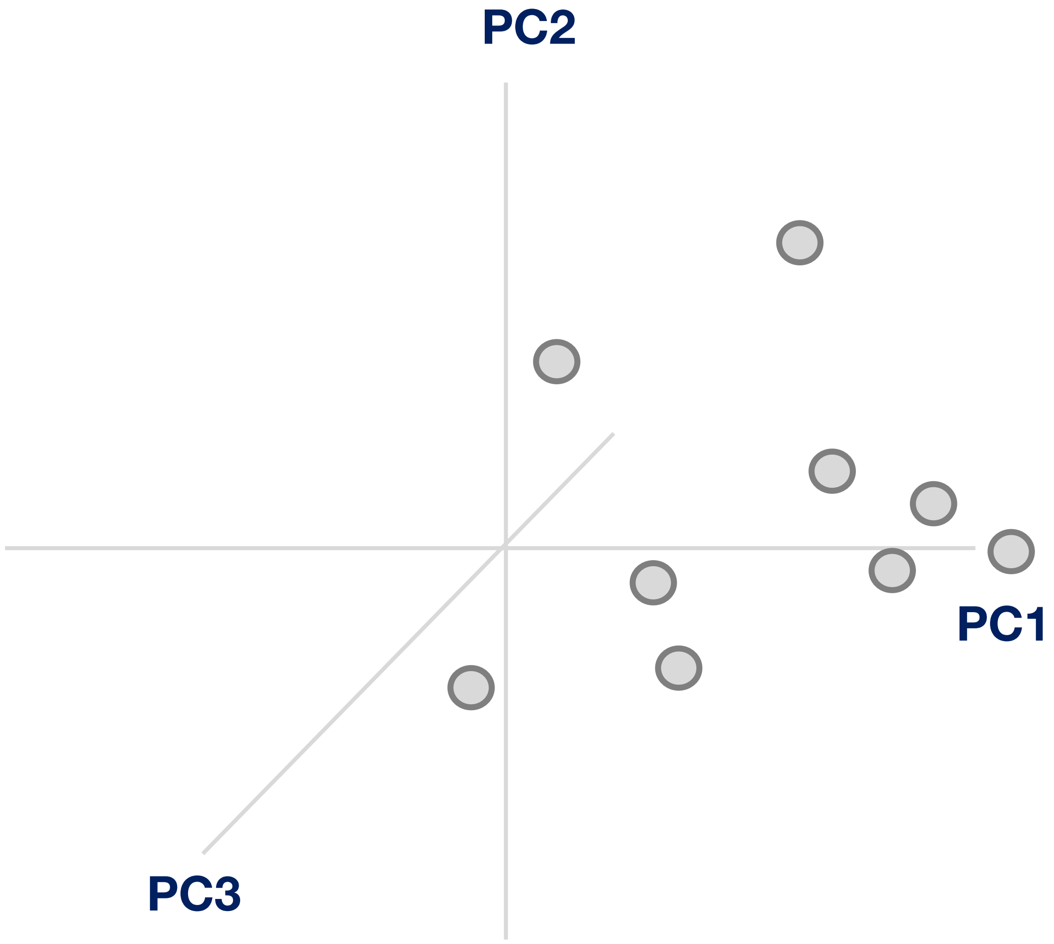
The projection (A’) of a point A on a particular line p is the point such that the line AA’ is perpendicular to p.



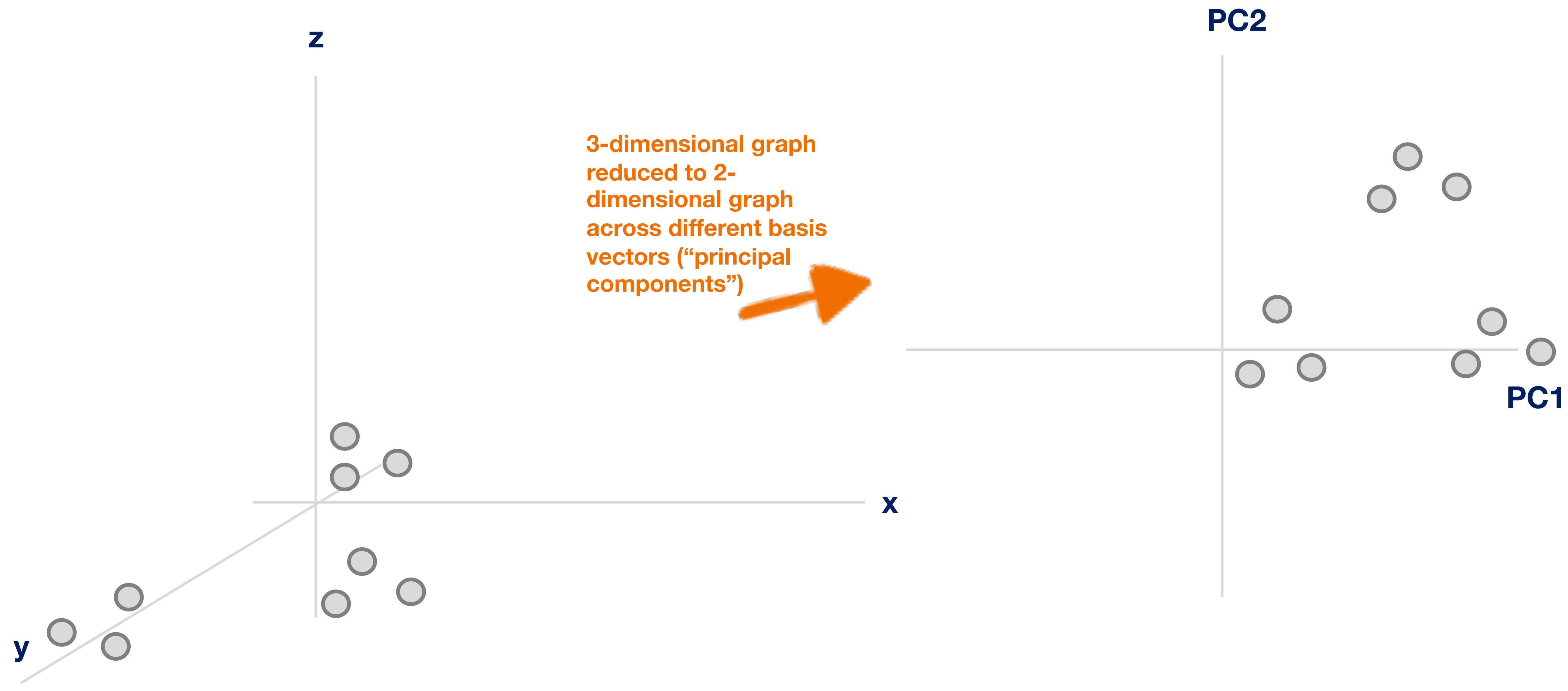
Principal Component Analysis



We can represent all data points along x,y,z axes in terms of new basis vectors PC1, PC2, and PC3.



Principal Component Analysis



Principal Component Analysis

How do we decide which PCs
to drop when reducing the
dimensionality of the data?

Principal Components

Think of these as new axes that we are orienting our data across.

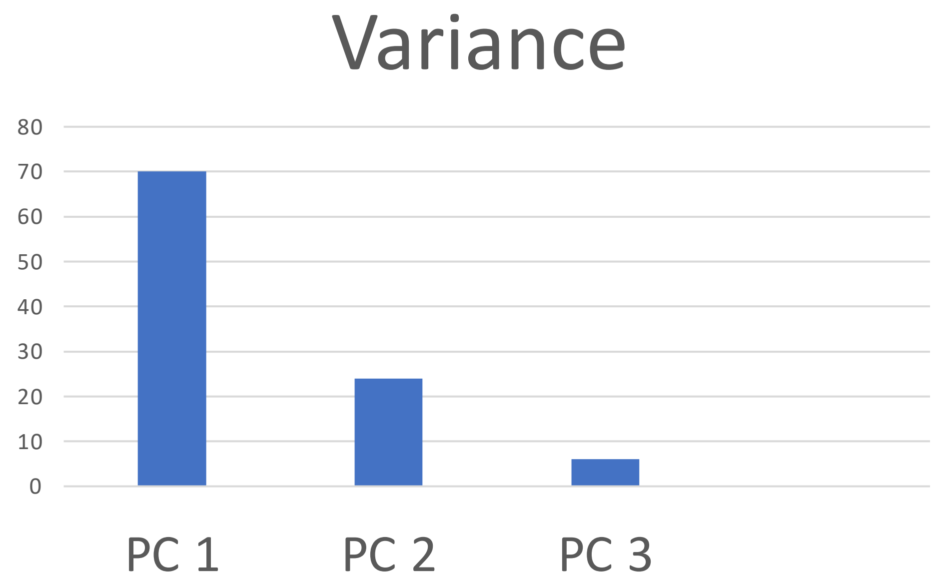
So instead of x,y, z, rather some linear combination of them.

They are done such that each principal component is uncorrelated with the others, so that translation across each component indicates different information. **So, they represent directions of maximal variance.**

This allows differences between data points to become more prominent

How do we decide which PCs to remove when reducing the dimensionality of the data?

Represents percentage of variance for each PC. Notice how PC1 has the most and it drops after that.

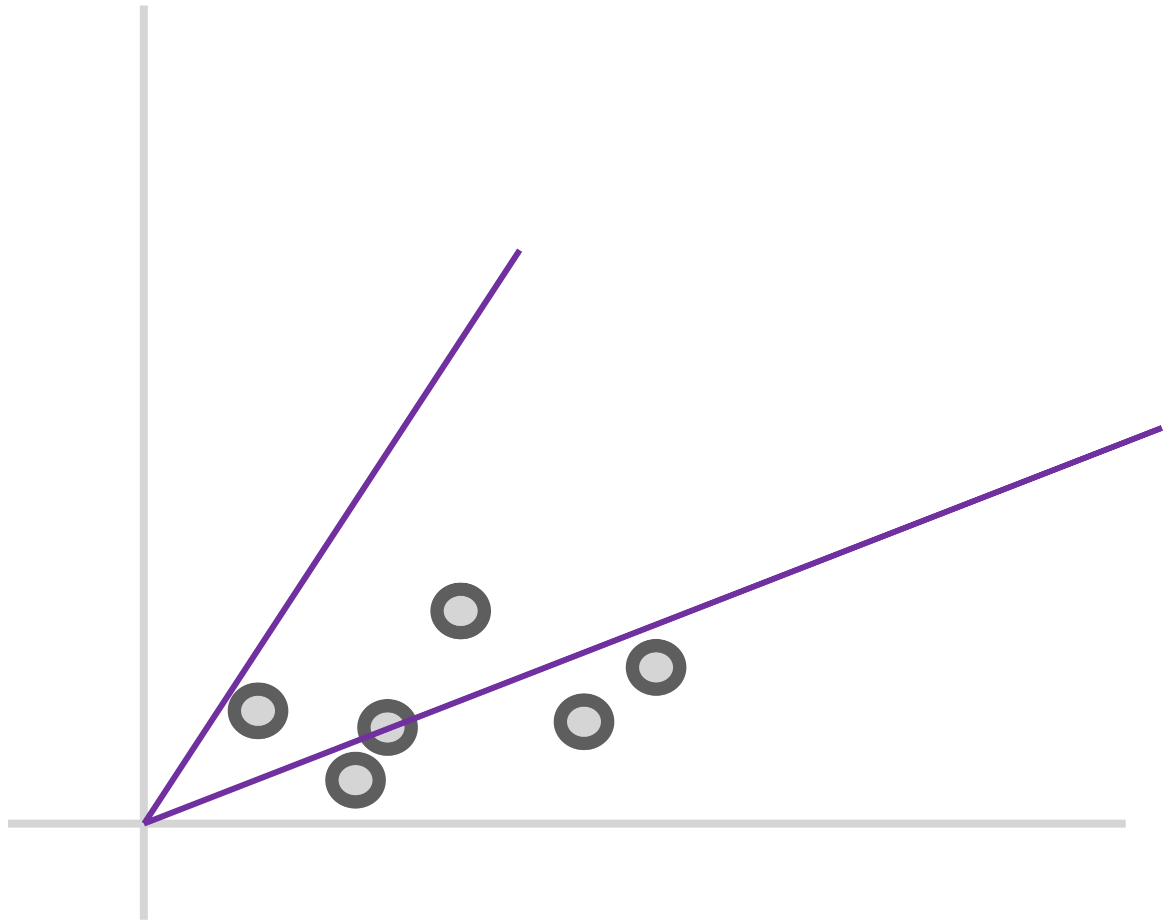


Since PC3 accounts for a very small percentage of overall variance, we can remove it. This is how PCA reduces dimensionality

Principal Component Analysis

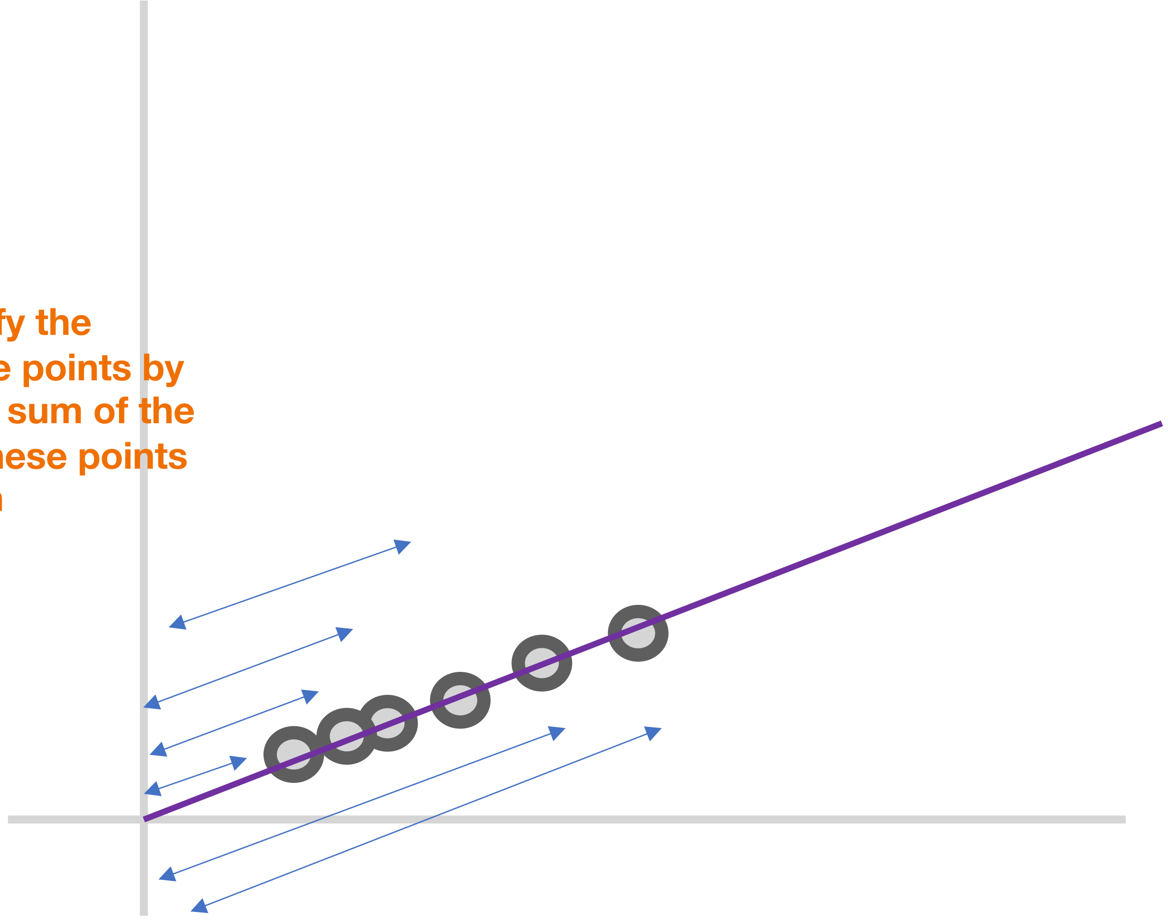
How do we decide the PCs?

Principal Component Analysis



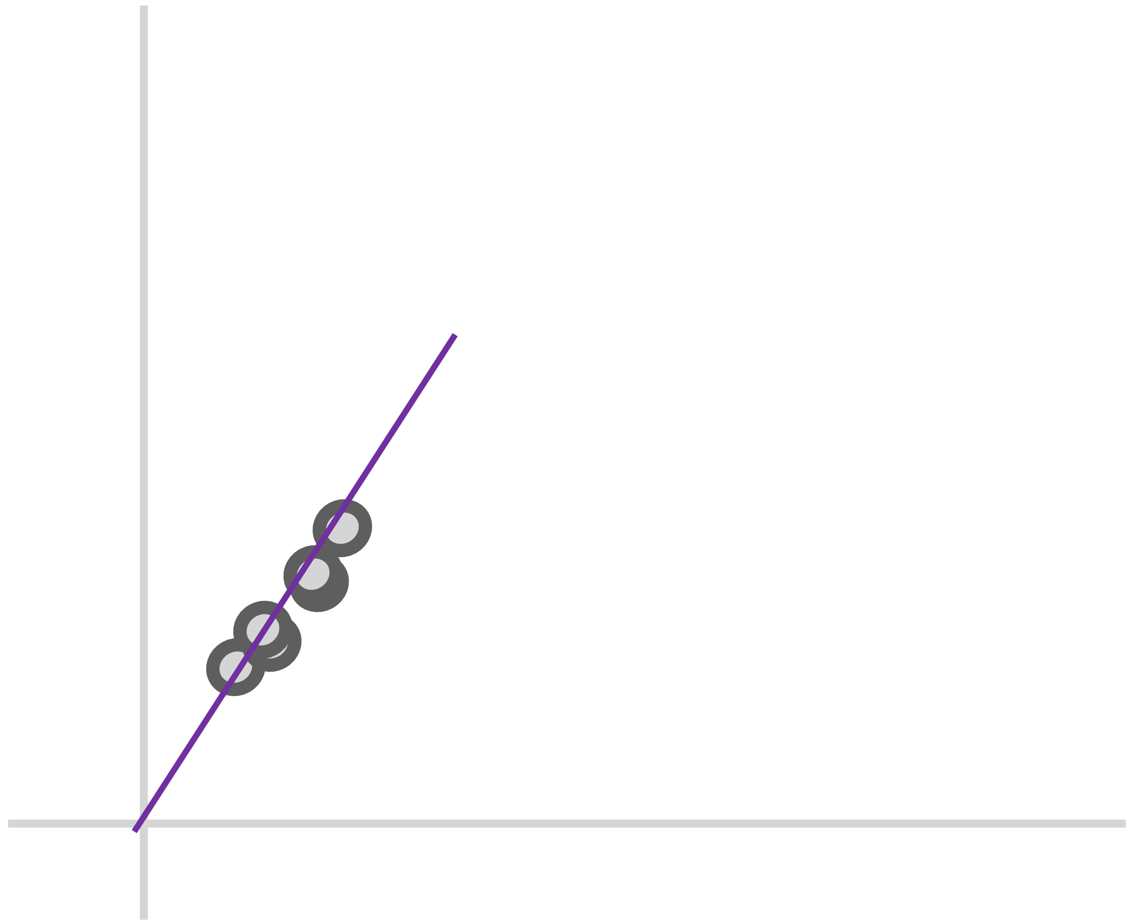
Principal Component Analysis

We can quantify the "spread" of the points by measuring the sum of the distances of these points from the origin



Notice how the points spread out from each other and from the origin.

Principal Component Analysis



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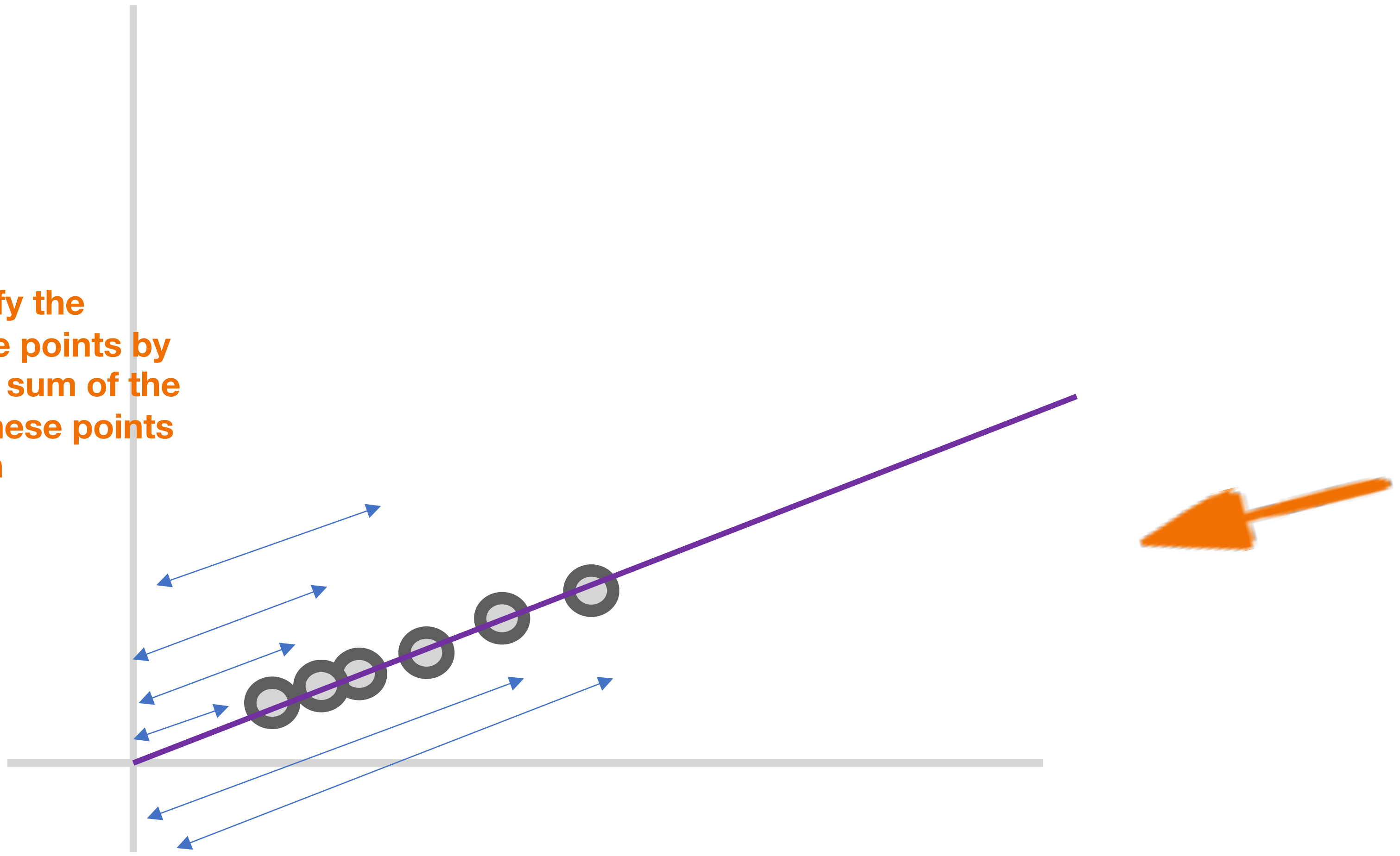

1st base or "Principal Component 1". Line that maximizes sum of distances of projections of points from origin. In essence, maximizes variance of distribution.

Principal Component Analysis

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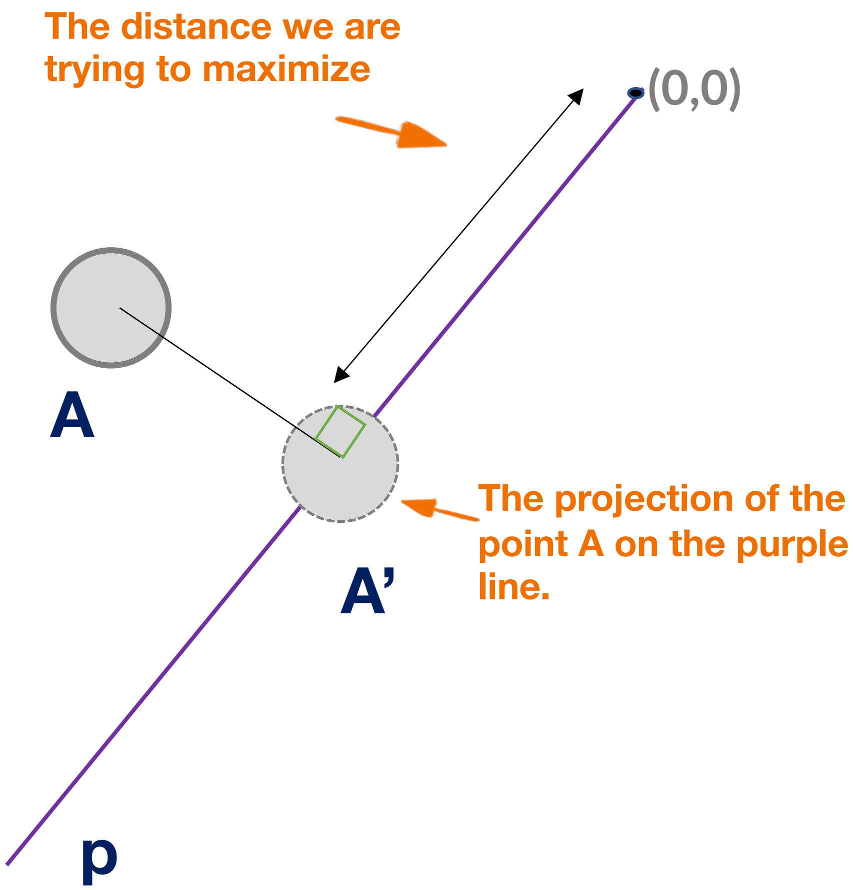
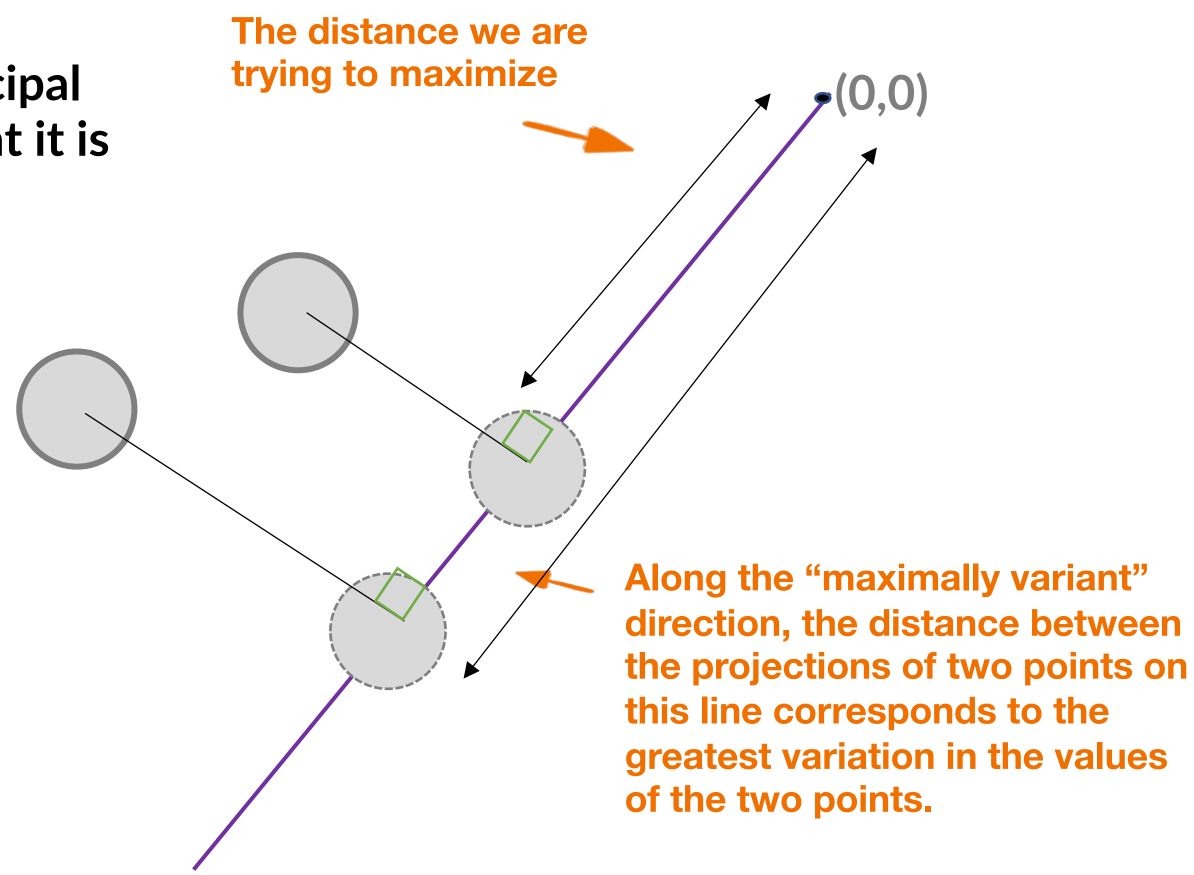
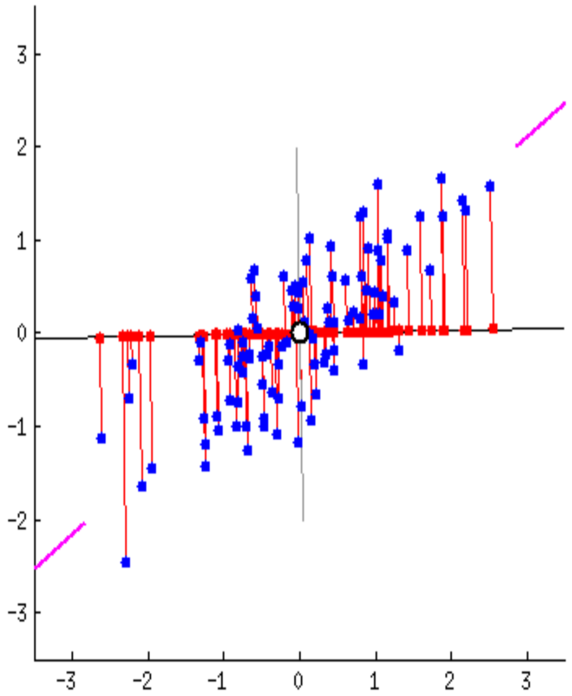


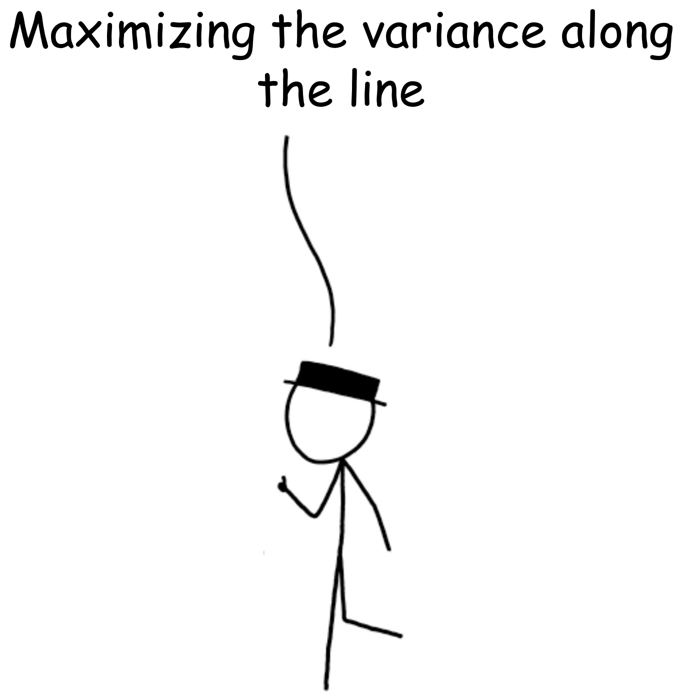
Principal Component Analysis

Idea behind this principal component line is that it is an axis along the "maximally variant" direction.



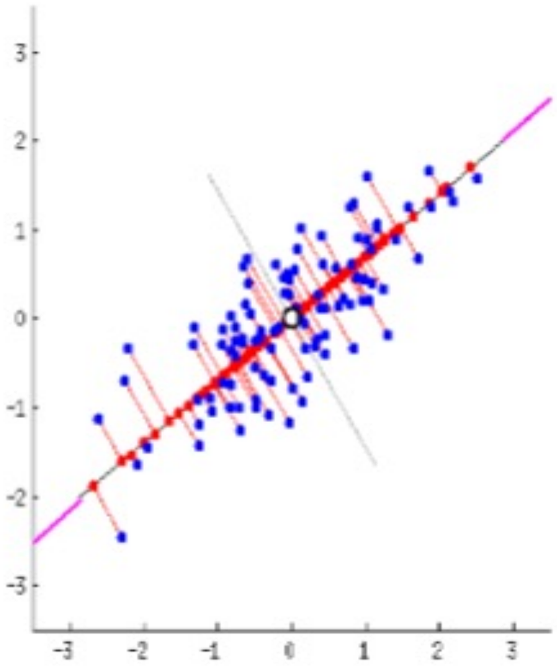
Principal Component Analysis

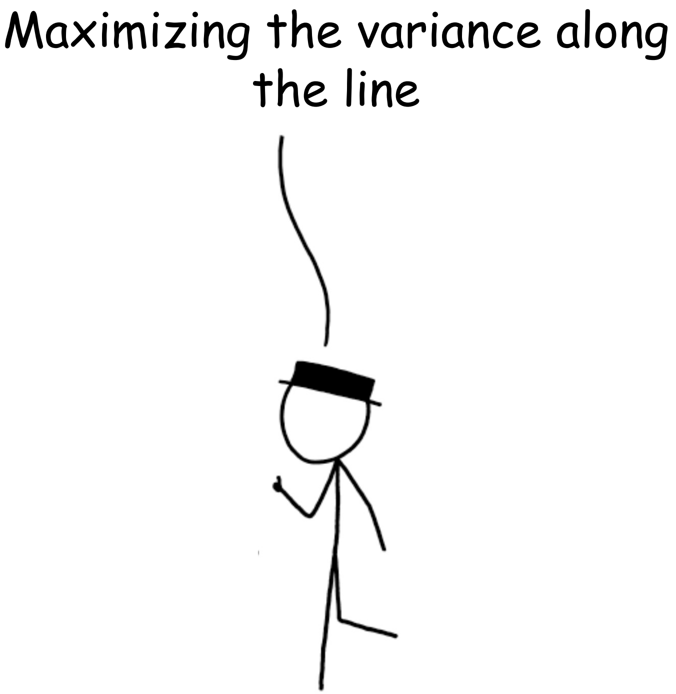




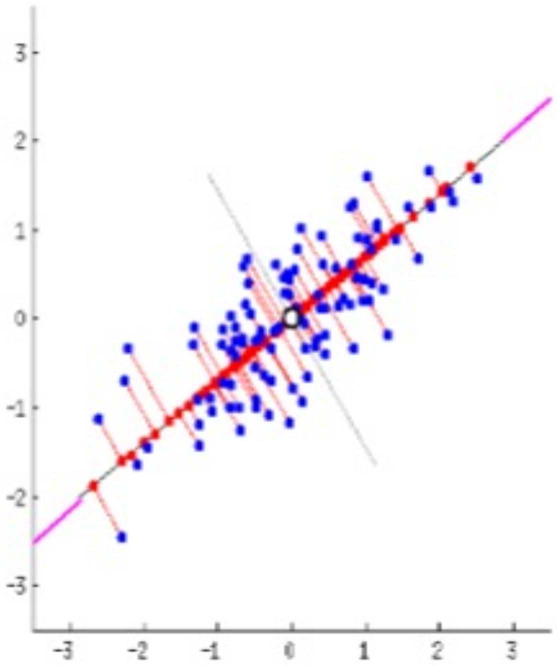
Built using https://gist.github.com/anonymous/7d888663c6ec679ea654287 15b99bfdd

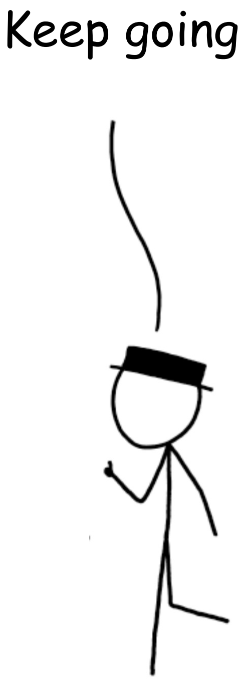
Principal Component Analysis





Principal Component Analysis





Principal Component Analysis

Standardization

Covariance Matrix Calculation

Eigenvector Calculation

Form Principal Components and Build Graph

Standardization

Individual	Height (cm)	Weight (kg)	Income ($)	Number of Children
Person A	165	65	60,000	2
Person B	168	63	100,000	5
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Compare the data of each of the 4 columns. How do they differ numerically?

Standardization

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Range	159-189	63-89	50,000-110,000	1-5
Variance	161.76	135.87	564166666	2.7

Compare the data of each of the 4 columns. How do they differ numerically?

Their range varies drastically. Consequently, their variances are very different.

Standardization

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Range	159-189	63-89	50k-100k	1-5
Variance	161.76	135.87	564166670	2.7

If this is not addressed, some of the feature columns will **dominate** over the other ones.

This can bias the results and final principal component analysis; making it difficult to view differences between values in one column compared to another.

So final graph may have the differences between the weights of various persons be miniscule.

Standardization

So, how do we adjust our data so these differences are not as drastic?

Standardization

Recap: we want to put different variables on the same scale.

This can mean many things from giving them the same mean and standard deviation, to keeping the range consistent, and so on.

Here, we will use a method called **z-scoring.**

$$z = \frac{value - mean}{standard\ deviation}$$

The rescaled distribution will have a mean of 0 and standard deviation of 1

Note: it does not mean the new data follow Normal distribution

Principal Component Analysis

Standardization

Covariance Matrix Calculation

Eigenvector Calculation

Form Principal Components and Build Graph

Covariance Matrix Calculation

Covariance is really just a measure of how **correlated** two variables/features are.

If your covariance is positive, that means there's a **positive correlation.**

If your covariance is positive, that means there's a **negative correlation.**

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

Covariance Matrix Calculation

Review: Lecture 7; feature engineering

Make new features with high variance.

Pick new features with low correlation to other features.

Covariance Matrix Calculation

Can measure this correlation using **covariance.** If covariance is **positive,** then features are correlated in the sense they both increase together. If covariance is **negative,** then features are inversely correlated.

$$\begin{bmatrix} Cov(x,x) & Cov(x,y) & Cov(x,z) \\ Cov(y,x) & Cov(y,y) & Cov(y,z) \\ Cov(z,x) & Cov(z,y) & Cov(z,z) \end{bmatrix}$$

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

Principal Component Analysis

Standardization

Covariance Matrix Calculation

Eigenvector Calculation

Form Principal Components and Build Graph

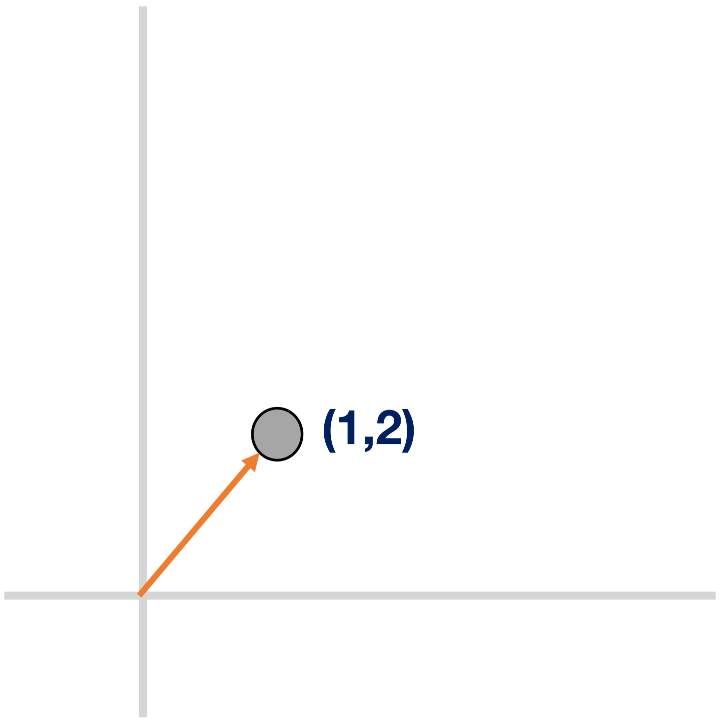
Eigenvector Calculation

We can think of matrices as **transformations** of vectors.

When you multiply a matrix with a vector; two things happen:

1. It **scales** the vector.
2. It **rotates** the vector

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$



Eigenvector Calculation

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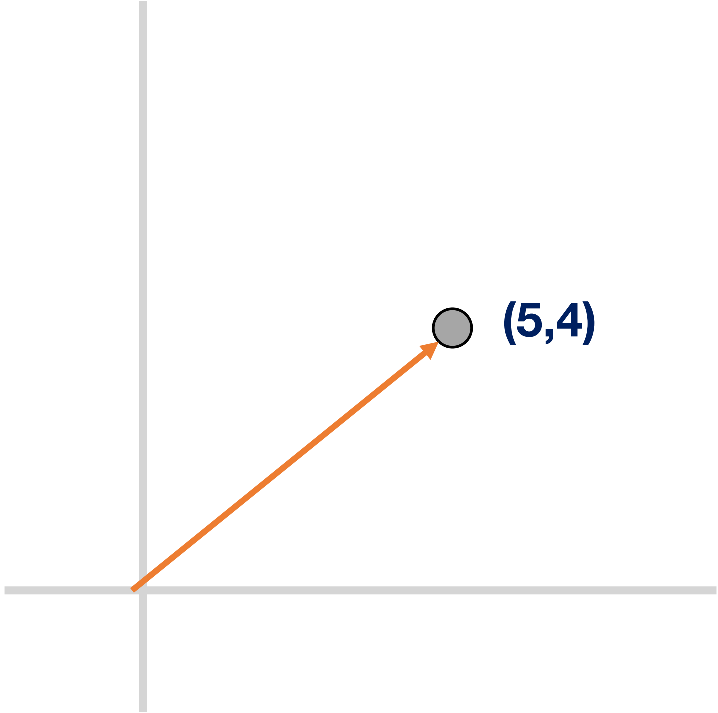
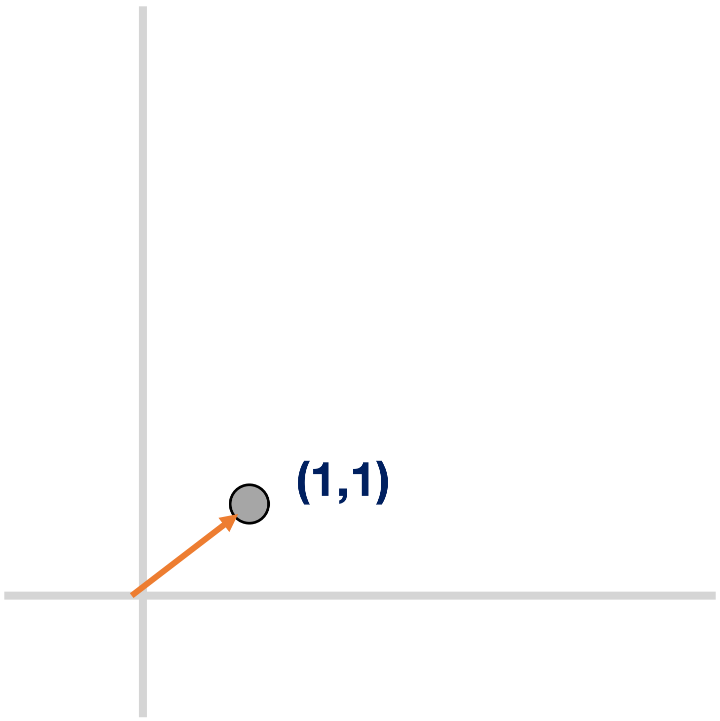


Eigenvector Calculation

Eigenvectors are characteristic vectors specific to a matrix or transformation.

Graphically speaking, when you multiply a matrix with its specific eigenvectors, the eigenvectors **don't get rotated, only scaled.**

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$



Eigenvector Calculation

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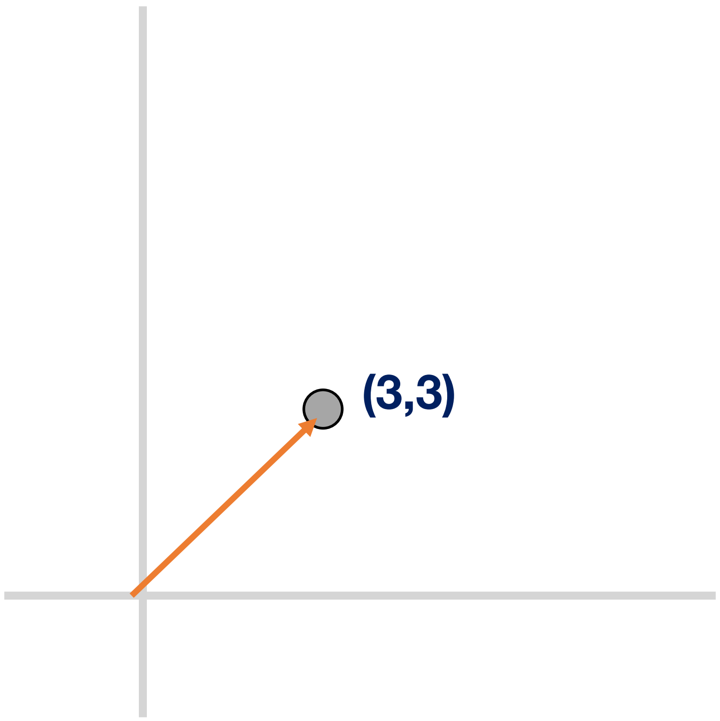
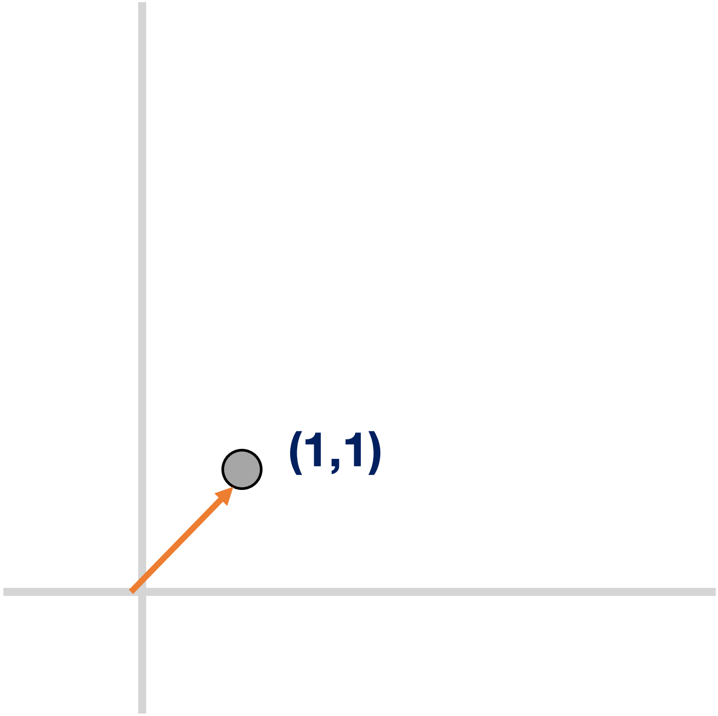
Graphically speaking, when you multiply a matrix with its specific eigenvectors, the eigenvectors **don't get rotated, only scaled.**

The factor by which an eigenvector is scaled is called its eigenvalue

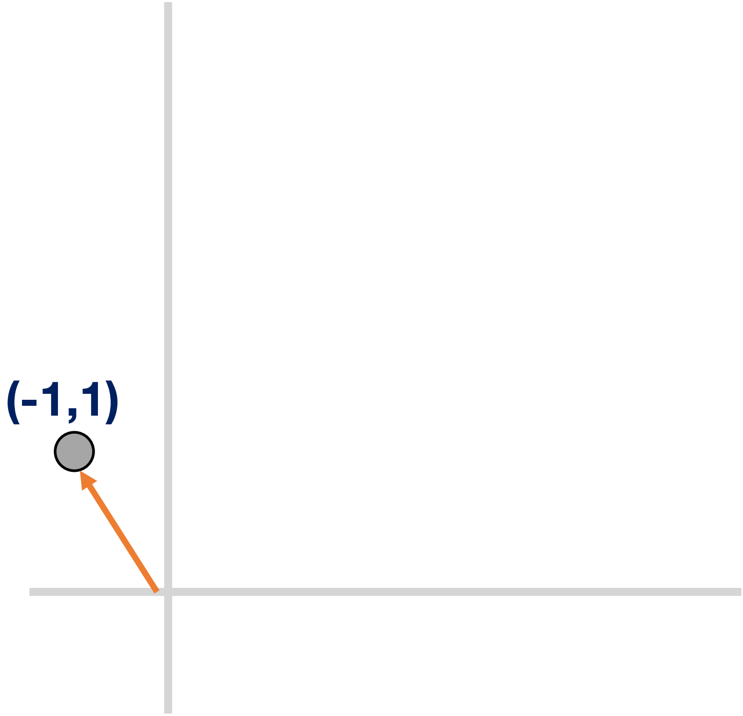
$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$



Eigenvector Calculation

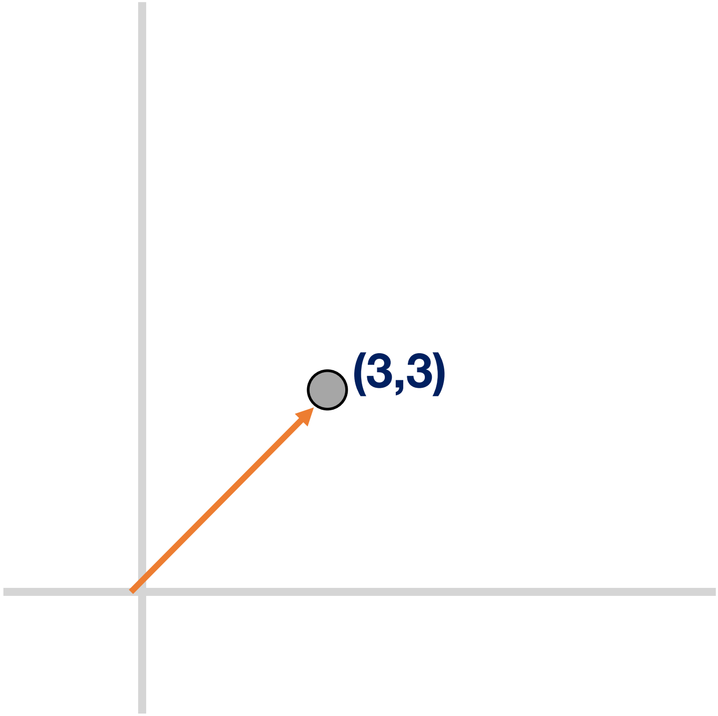


$$\begin{bmatrix}1 & 2\\2 & 1\end{bmatrix}\begin{bmatrix}1\\1\end{bmatrix} = \begin{bmatrix}3\\3\end{bmatrix} = 3\begin{bmatrix}1\\1\end{bmatrix}$$



$$\begin{bmatrix}1 & 2\\2 & 1\end{bmatrix}\begin{bmatrix}-1\\1\end{bmatrix} = \begin{bmatrix}1\\-1\end{bmatrix} = -1\begin{bmatrix}-1\\1\end{bmatrix}$$

Eigenvector Calculation



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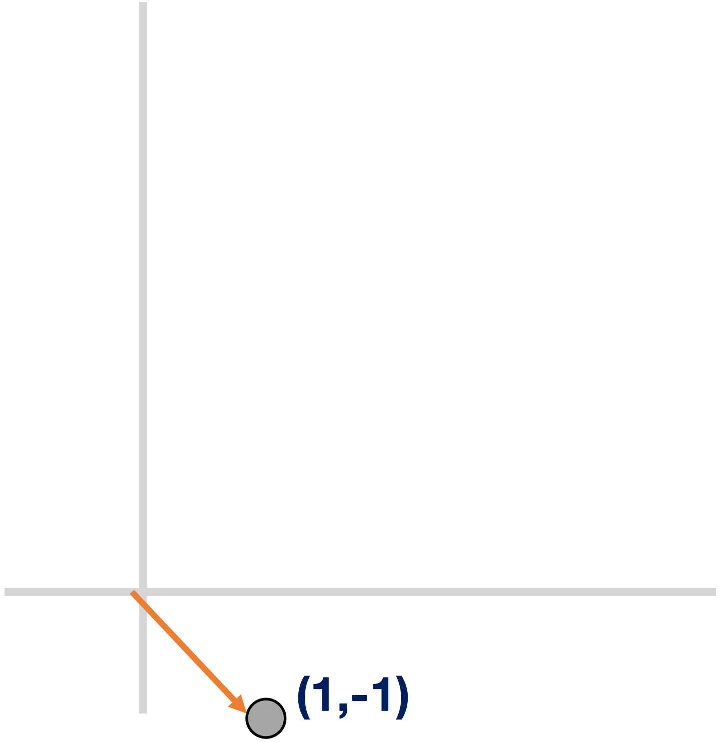
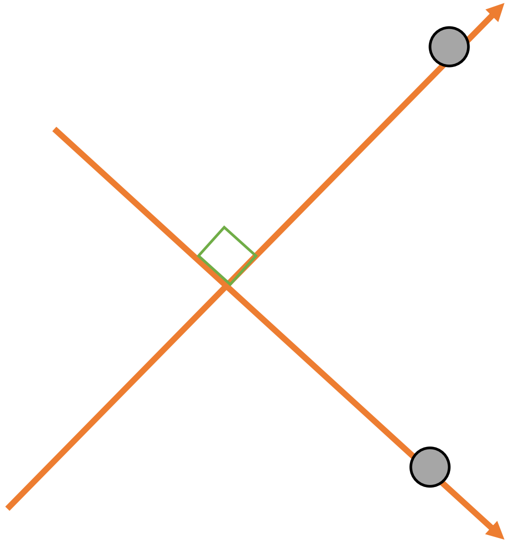


$$\begin{bmatrix}1 & 2\\2 & 1\end{bmatrix}\begin{bmatrix}-1\\1\end{bmatrix} = \begin{bmatrix}1\\-1\end{bmatrix} = -1\begin{bmatrix}-1\\1\end{bmatrix}$$

Eigenvector Calculation

The two eigenvectors are perpendicular to each other!

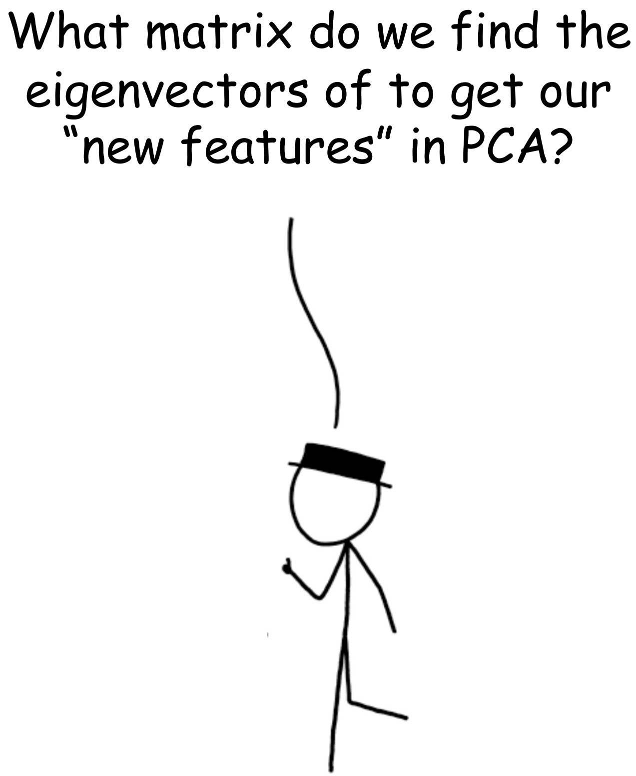


Eigenvectors act as basis vectors!

Every point in 2-D can be expressed as some combination of (1,1) and (-1,1).

Eigenvector Calculation

Eigenvector Calculation



Eigenvector Calculation

By calculating the eigenvectors of the covariance matrix, we can get our **principal components.**

We use the eigenvectors to create a basis for the graph. These basis vectors represent the principal components.

Since these are eigenvectors of the **covariance matrix**, they represent **directions of maximal variance.**

$$A = \begin{bmatrix} Cov(x,x) & Cov(x,y) & Cov(x,z) \\ Cov(y,x) & Cov(y,y) & Cov(y,z) \\ Cov(z,x) & Cov(z,y) & Cov(z,z) \end{bmatrix}$$

$$Av = \lambda v$$

v is the eigenvector and lambda is the eigenvalue

Eigenvector Calculation

$$Av = \lambda v$$

$$Av - \lambda v = 0$$

$$(A - \lambda)v = 0$$

$$|A - \lambda| = 0$$

$$A = \begin{bmatrix} Cov(x,x) & Cov(x,y) & Cov(x,z) \\ Cov(y,x) & Cov(y,y) & Cov(y,z) \\ Cov(z,x) & Cov(z,y) & Cov(z,z) \end{bmatrix}$$

When you find the root of the resulting polynomial, you will find all the possible eigenvalues. For each eigenvalue, plug it into the original equation to find the corresponding eigenvector v.

Principal Component Analysis

Standardization

Covariance Matrix Calculation

Eigenvector Calculation

Form Principal Components and Build Graph

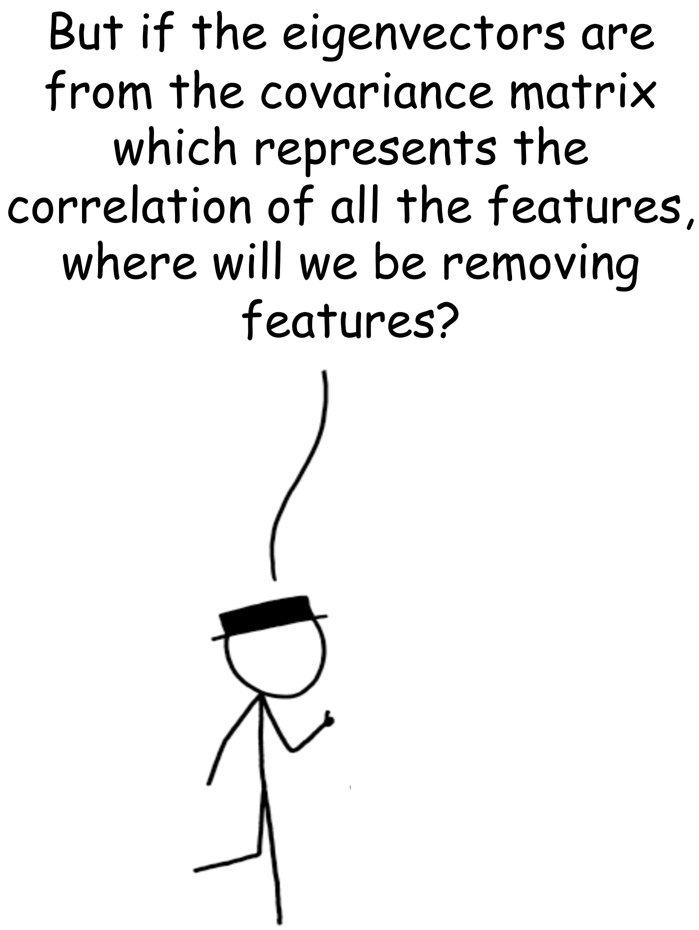
Form Principal Components and Build Graph

Let the three eigenvalues of the three eigenvectors $v_1, v_{2,}, v_3$ be $\lambda_1, \lambda_2, \lambda_3$ such that $\lambda_1 >= \lambda_2 >= \lambda_3$

Then, the principal components will be $v_1, v_{2,}, v_3$ and the variances they carry are in the ratio of $\lambda_1, \lambda_2, \lambda_3$

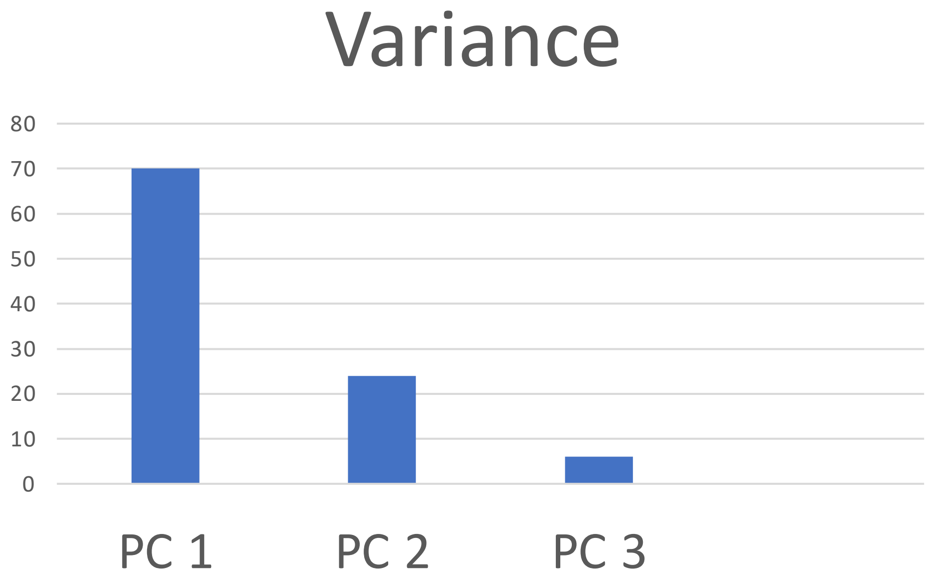
But if the eigenvectors are from the covariance matrix which represents the correlation of all the features, where will we be removing features?

Form Principal Components and Build Graph



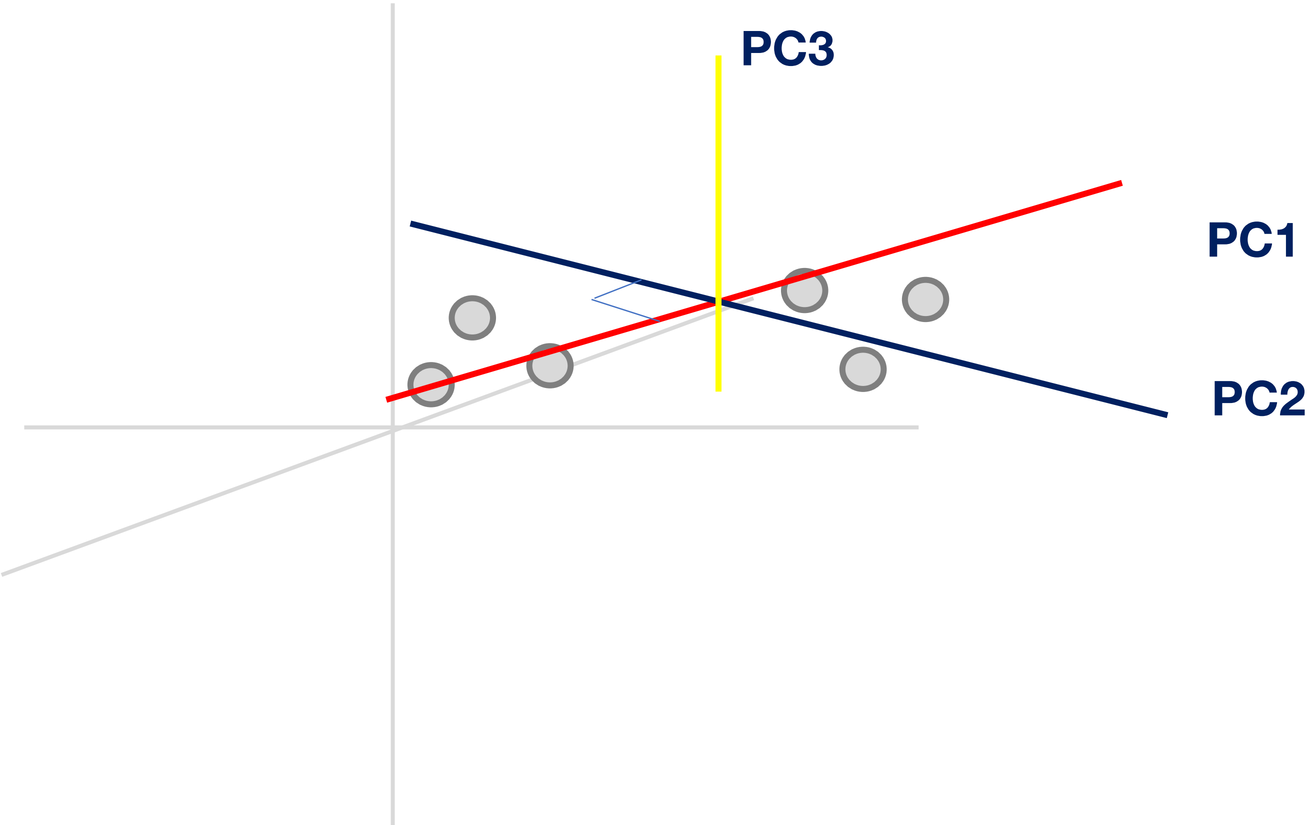
If the percentage of variance of a particular principal component is small enough, discard it. You've now removed a dimension! Form a new matrix which only has the eigenvectors/principal components you've selected.

Let this matrix be called your **Feature Vector.**



Now, it’s time to reorient the original data along these new axes

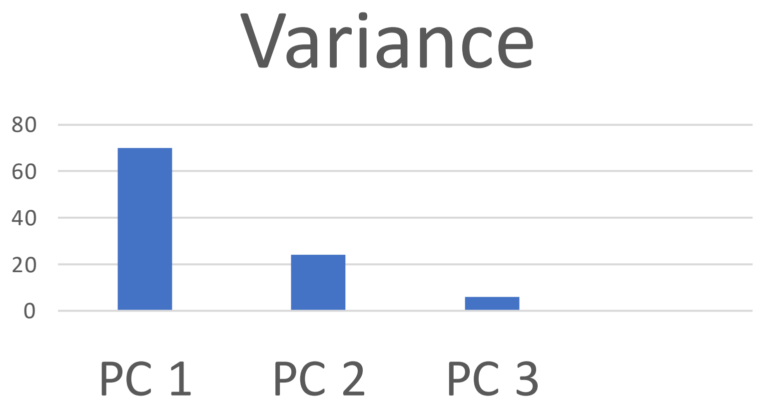
Form Principal Components and Build Graph

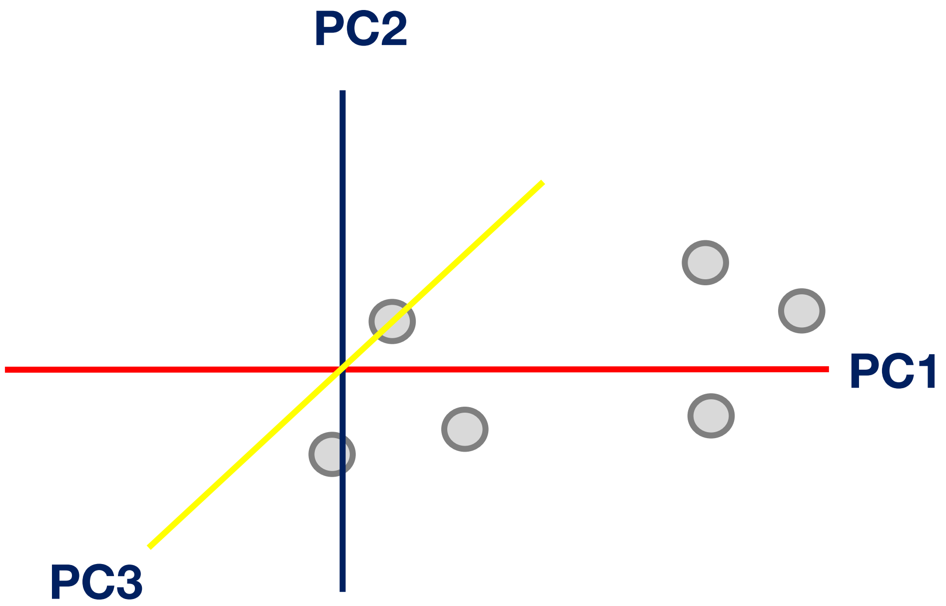


$$FinalDataSet = FeatureVector^T * StandardizedOriginalDataSet^T$$

Form Principal Components and Build Graph

The third dimension was removed as it did not contribute much in terms of variance





$$FinalDataSet = FeatureVector^T * StandardizedOriginalDataSet^T$$

Principal Component Analysis

Linear transformation of existing features

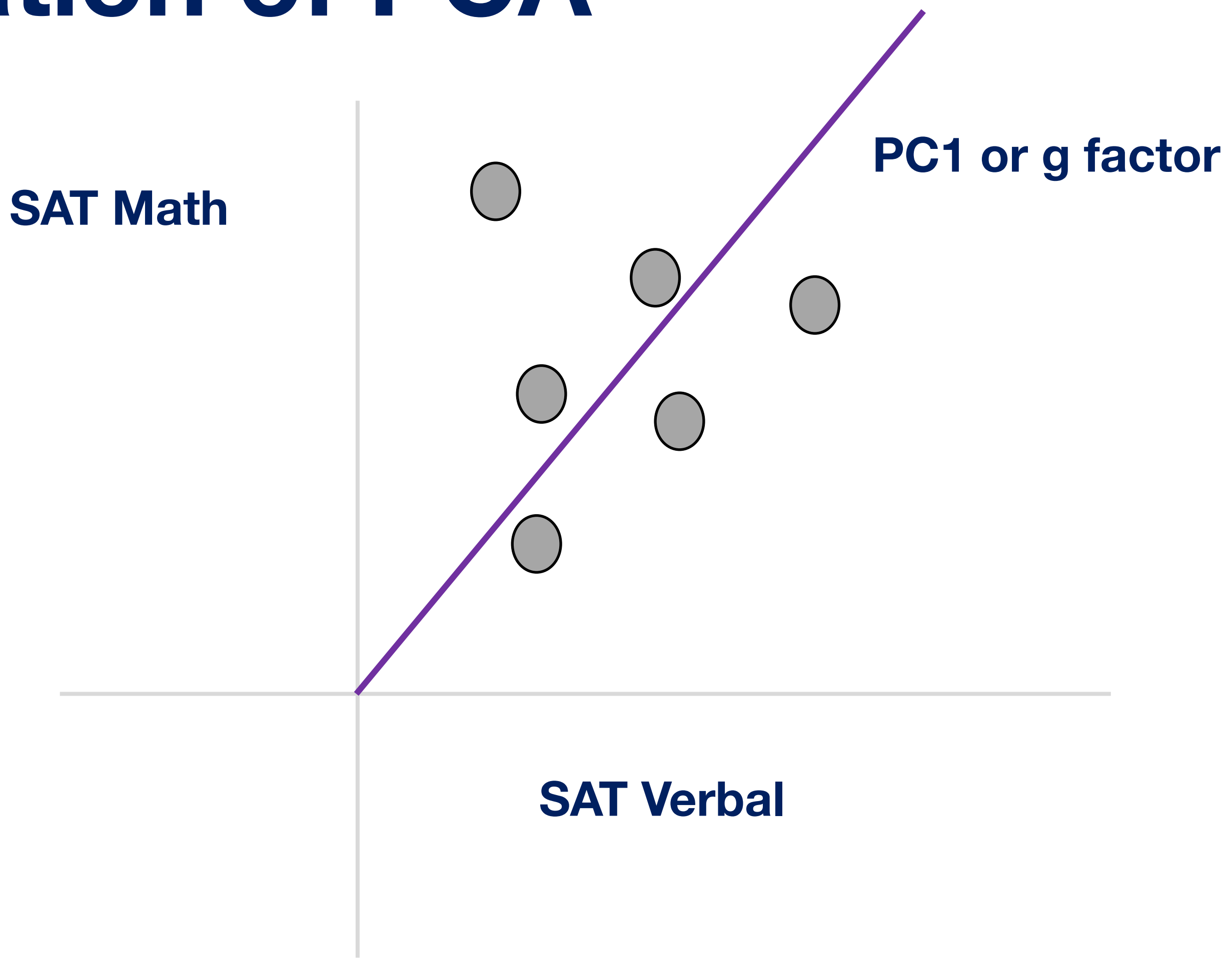
Each PC is selected to maximize the explained variance in this direction of the remain data

Dimensionality reduction is to remove dimensions with low variances

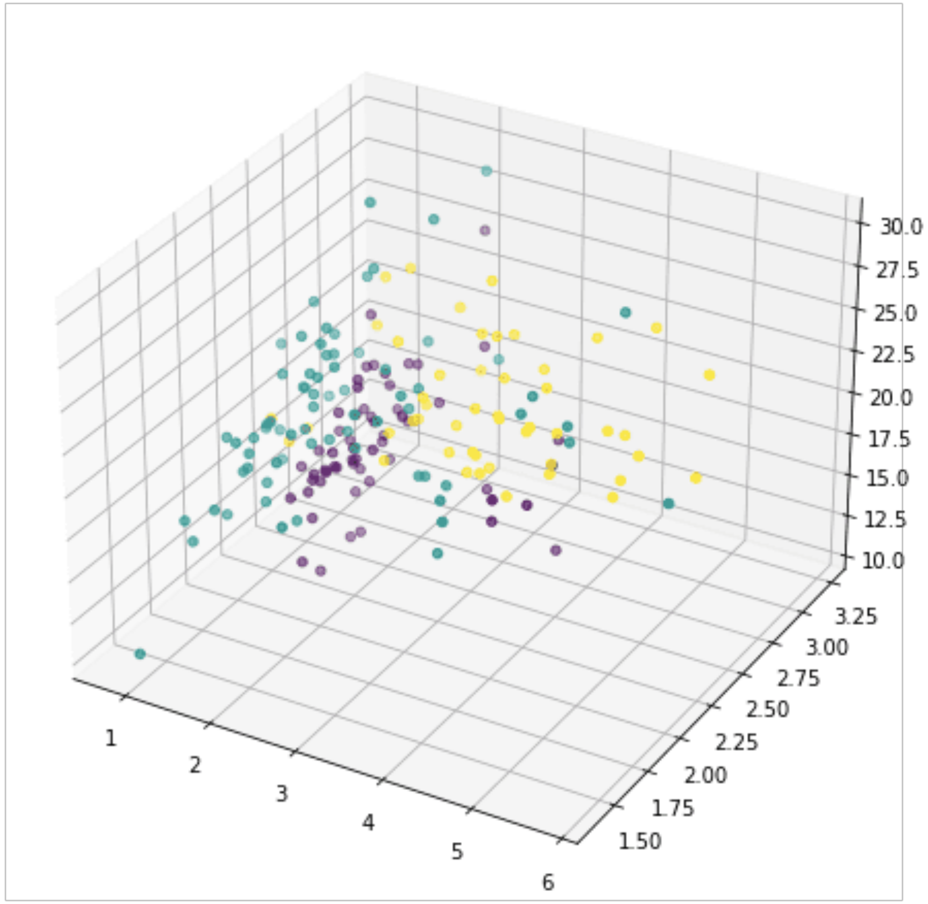
Tradeoff between dimensionality vs. info. loss

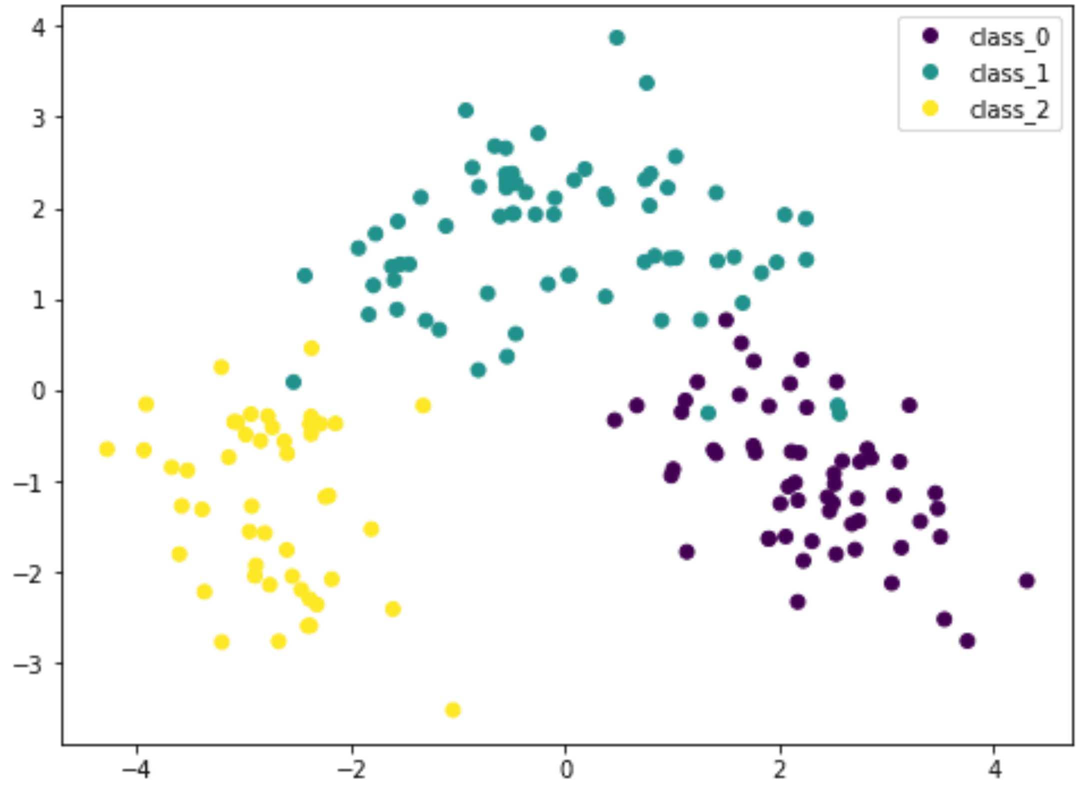
A real-world application of PCA

IQ testing!



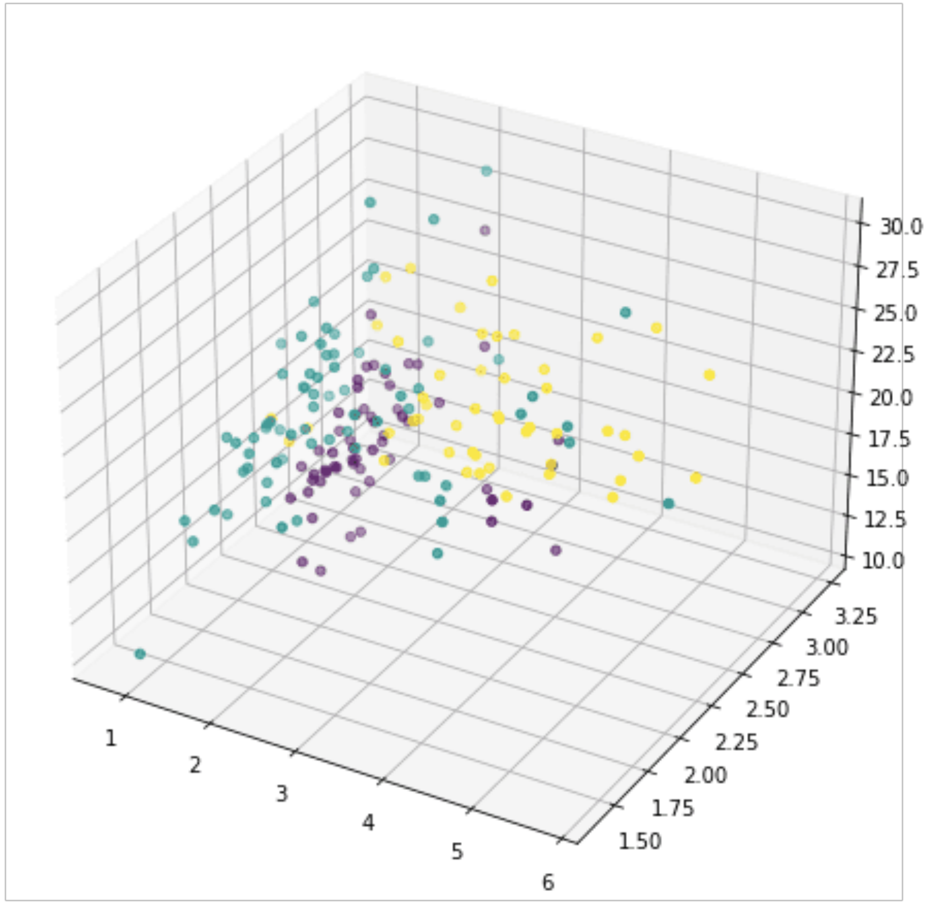
Data Visualization

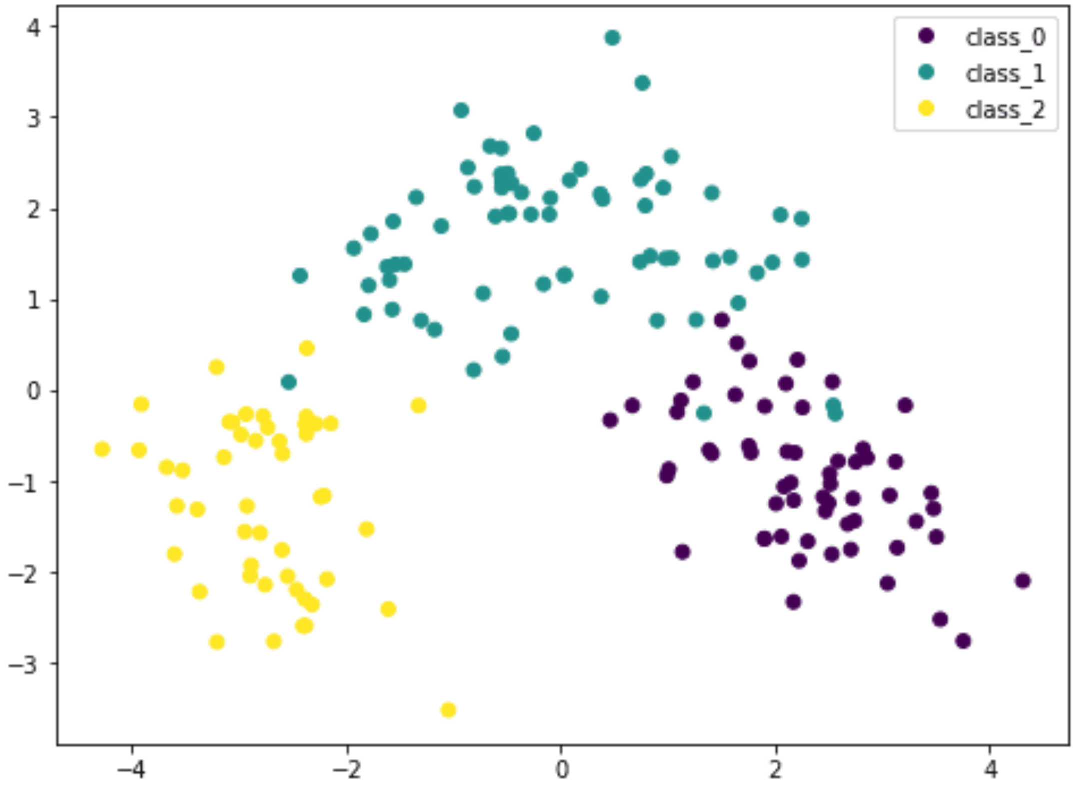




The wine dataset with 13 features and 3 classes.
Source: https://machinelearningmastery.com/principal-component-analysis-for-visualization/

Feature Extraction

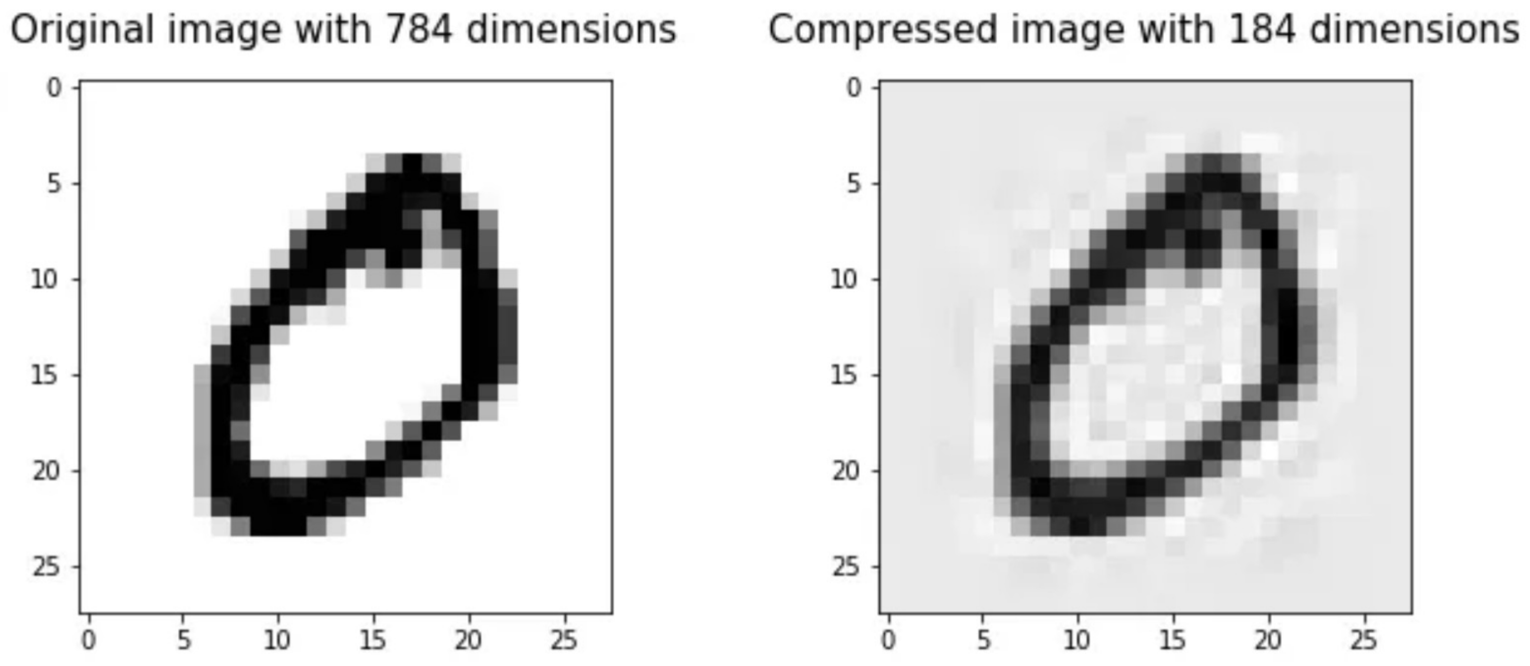




Q: feature extraction vs. feature selection?

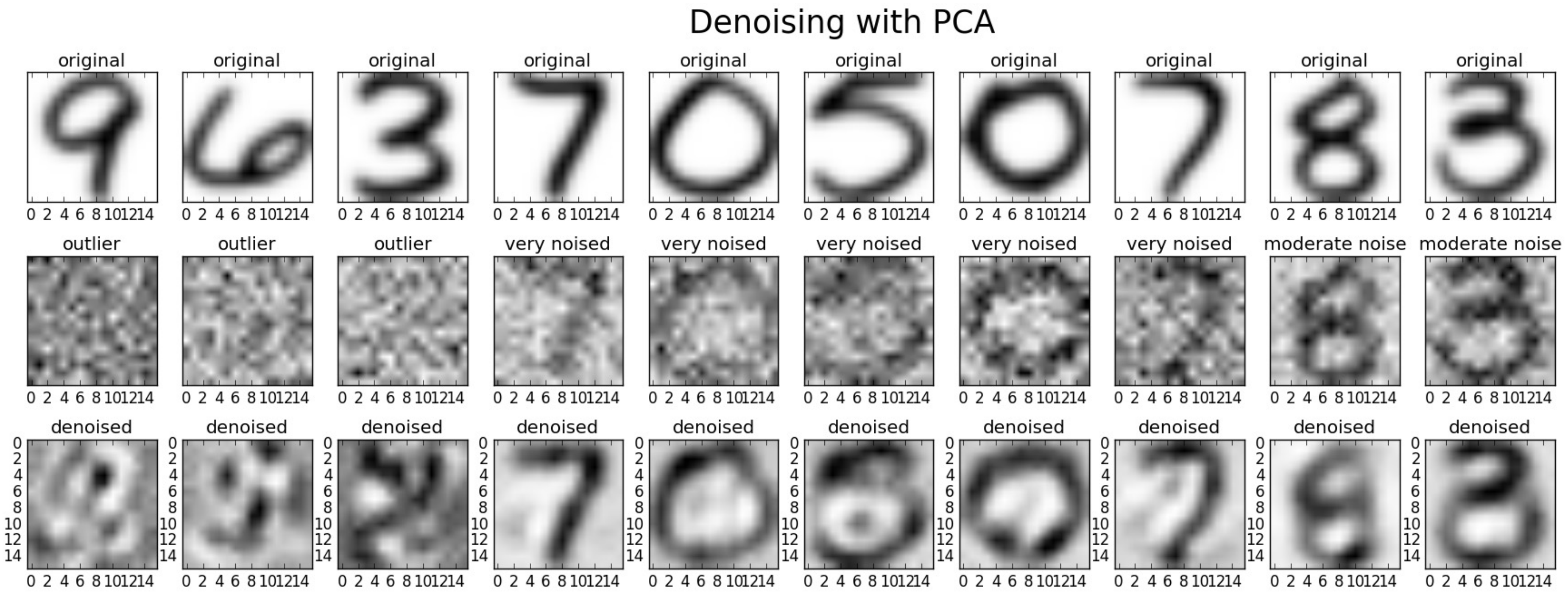
The wine dataset with 13 features and 3 classes.
Source: https://machinelearningmastery.com/principal-component-analysis-for-visualization/

Image Compression



Source: https://towardsdatascience.com/image-compression-using-principal-component-analysis-pca-253f26740a9f

Noise Reduction



Source: https://stats.stackexchange.com/questions/247260/principal-component-analysis-eliminate-noise-in-the-data

Unsupervised Learning

Clustering

Dimension reduction