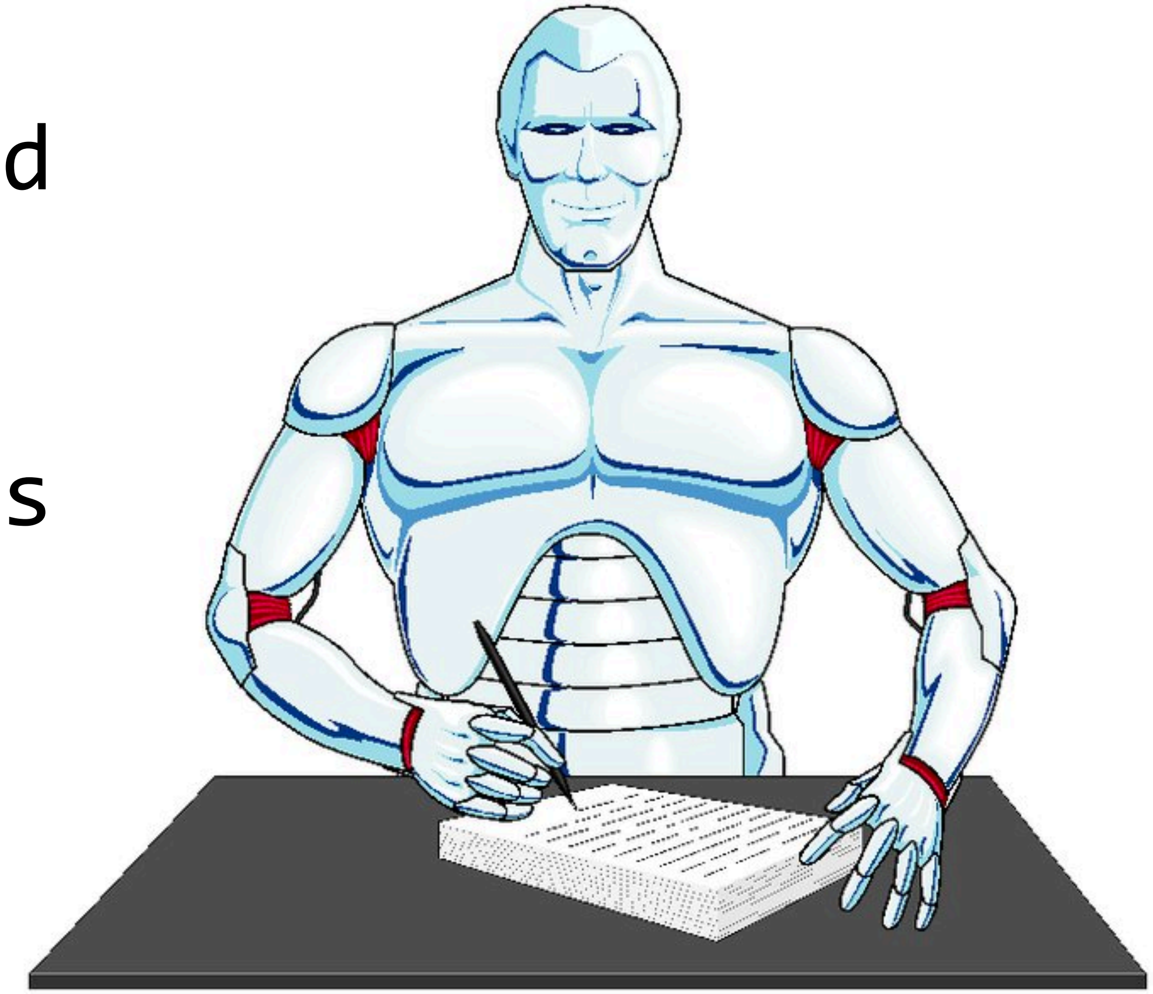
PRINCIPAL COMPONENTS ANALYSIS

11.30.2020

FINAL

* the final will be posted **next monday** (Dec. 7)

* it will be due (and this is a HARD deadline) on Monday, December 14 at 10:59 AM



FINAL

* the final will be SELF-TIMED (*honor system*!) for 4 hours (no proctorio, etc.)

  * your time starts when you first look at it, and you should stop working on it (& turn it in) 4 hours later

* it is **OPEN BOOK, OPEN DOCUMENTATION, & OPEN INTERNET**

  * but don’t discuss it with anyone else until you have both finished it

FINAL

* the final will cover all the topics we’ve touched on in class

* it will be EASIER THAN THE HOMEWORKS

  * i.e. the vast majority of you should finish in 4 hours

* good luck :)

PCA

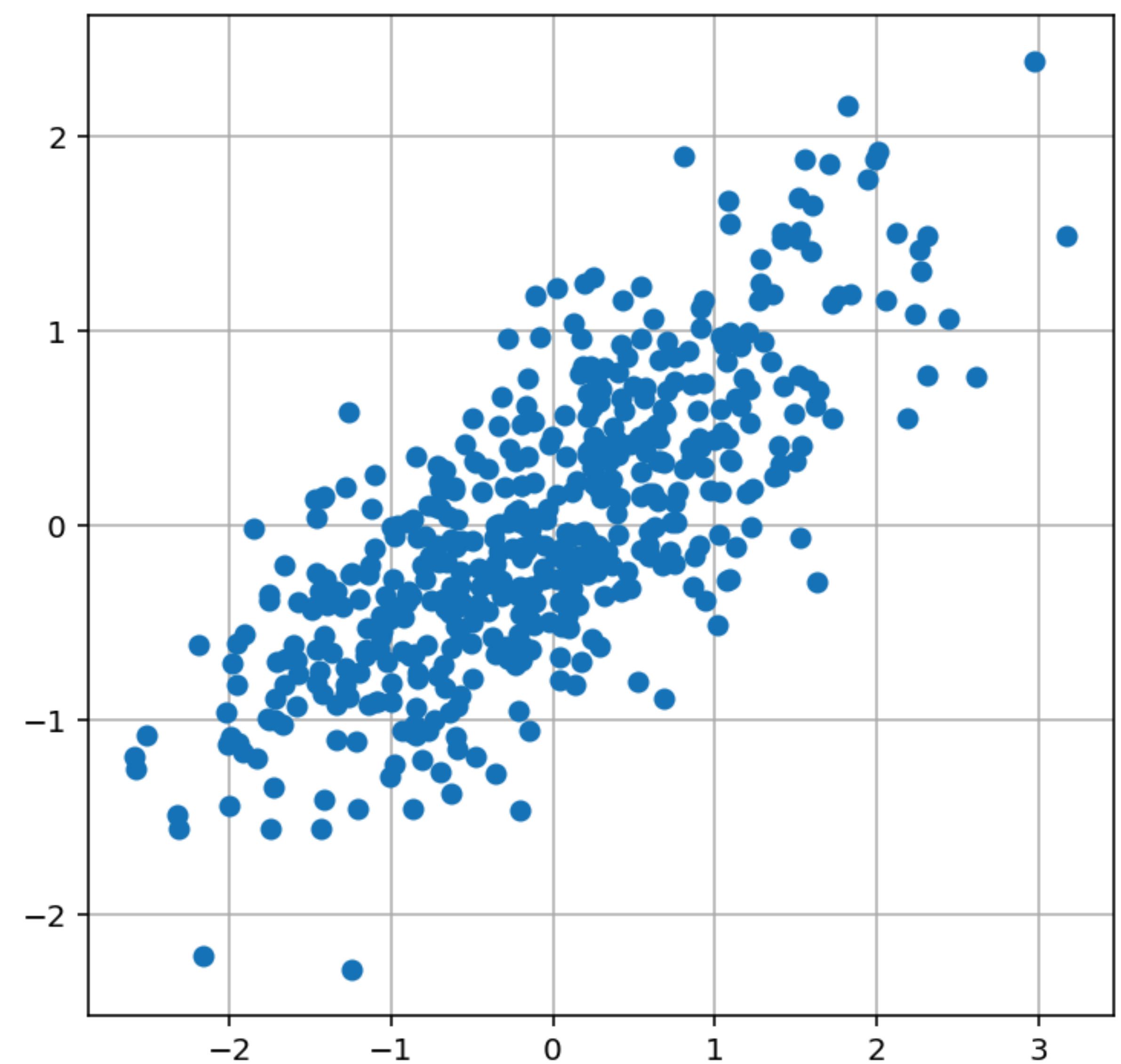
* **Principal Components Analysis** is an *unsupervised* method for finding structure in datasets

  * (This is different from regression & classification, which are examples of *supervised learning*. They learn a function f(X)=y. Here we only have X!)

PCA

* The typical explanation of PCA:

* PCA “fits an ellipse” to a cloud of datapoints



PCA

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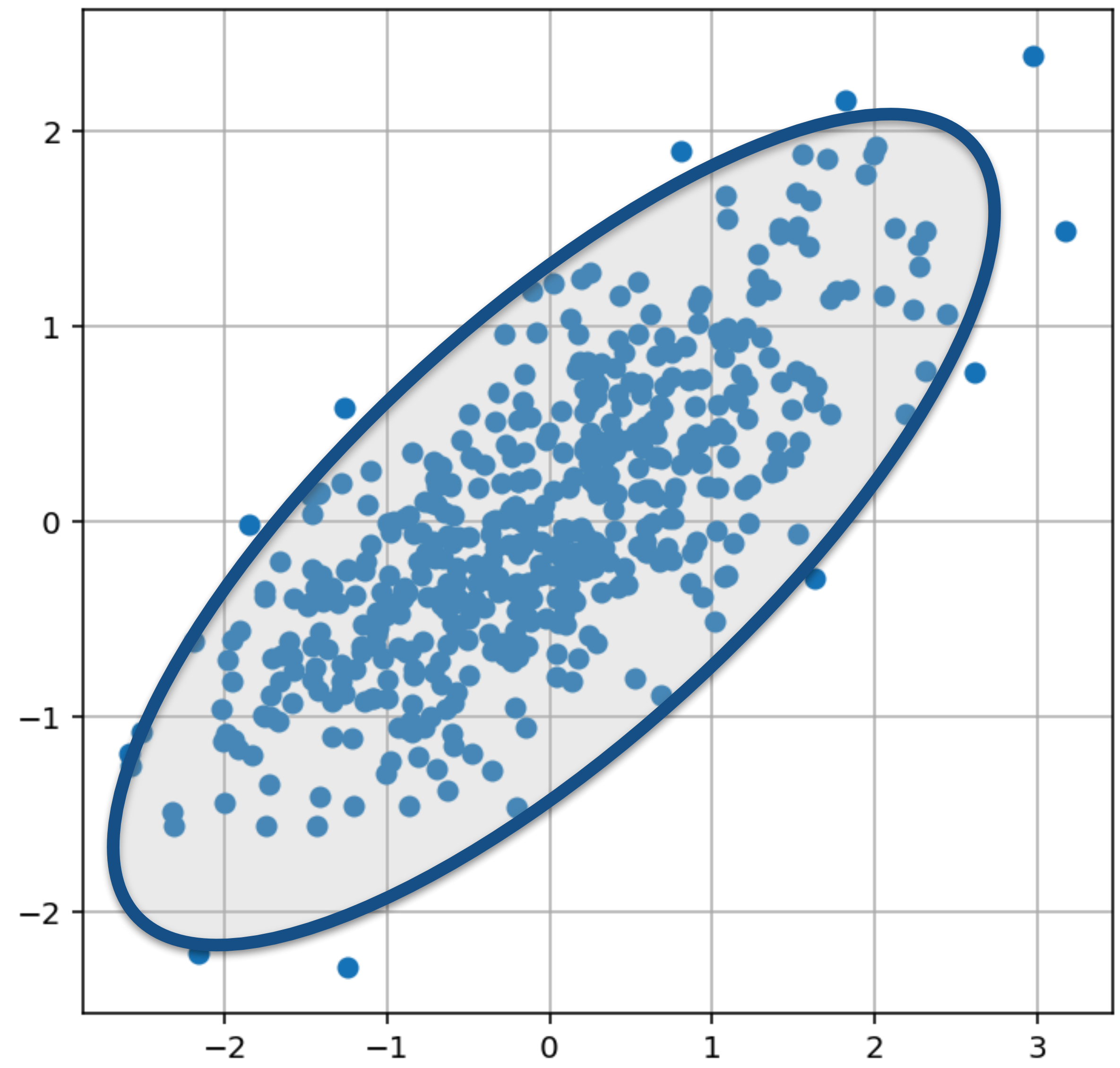
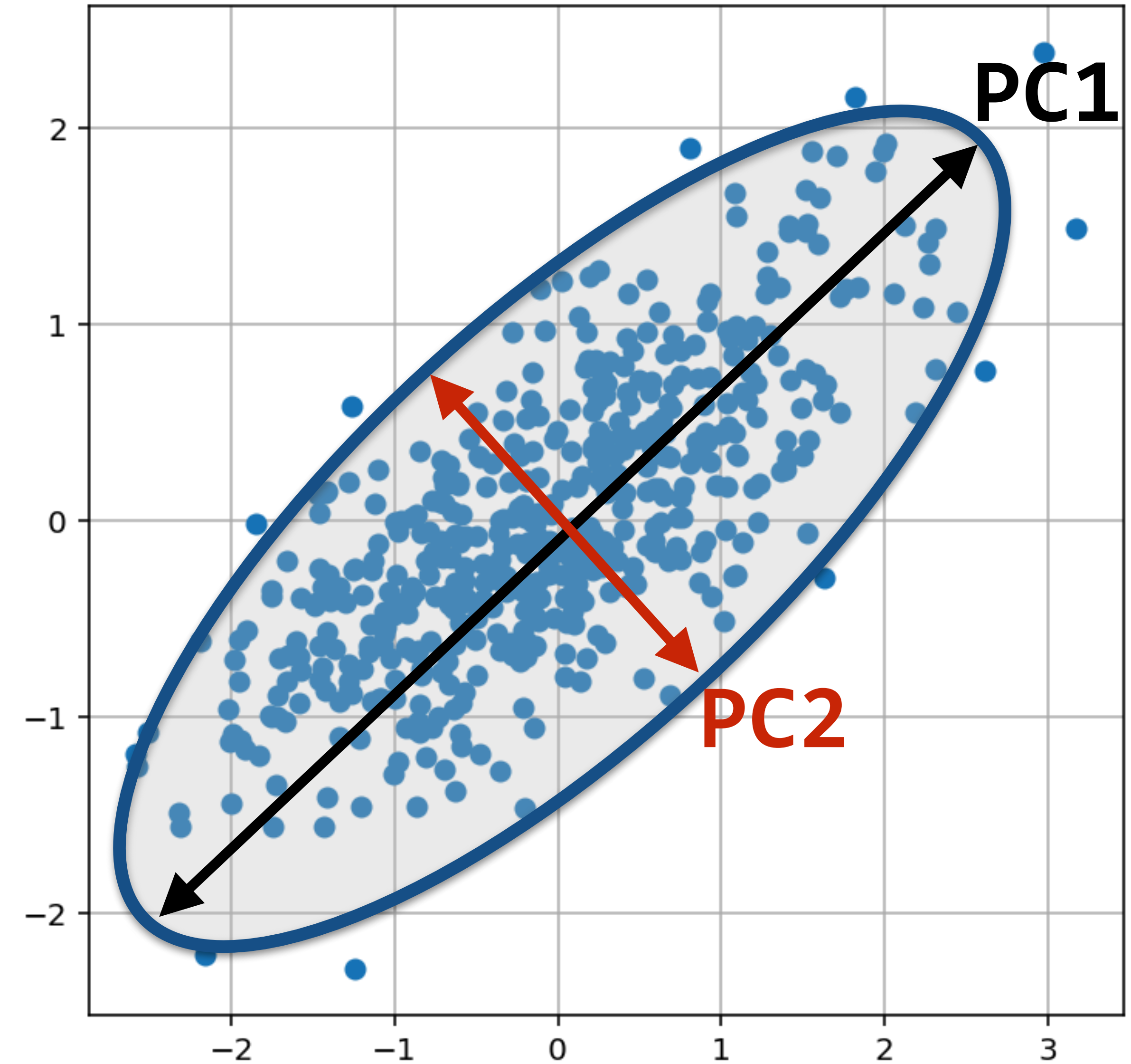


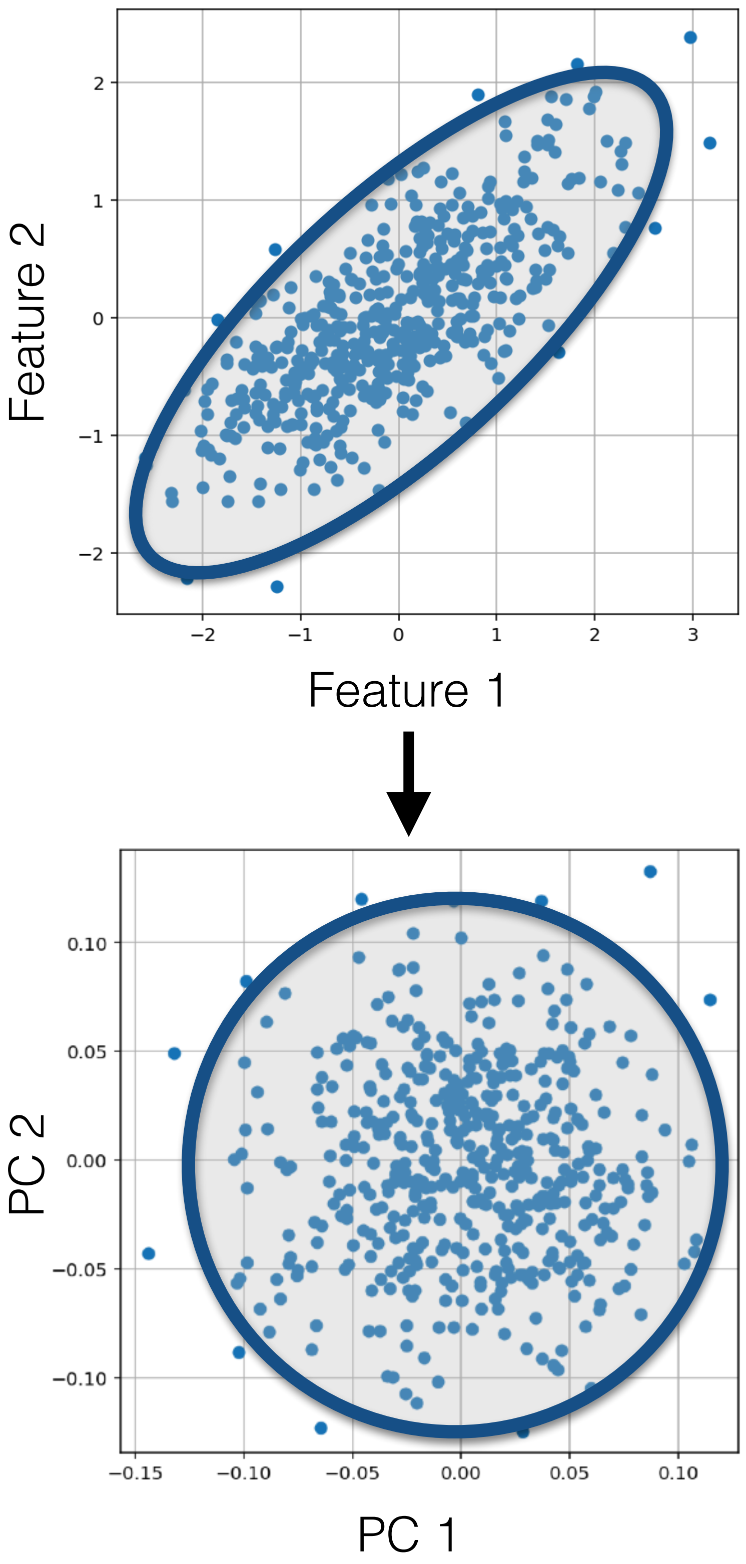
PCA

* The axes of the ellipse are the “principal components”



PCA

* It also gives you a way to *transform* the data so that the ellipse becomes a perfect circle



PCA

* But the key use case of PCA is *dimensionality reduction*

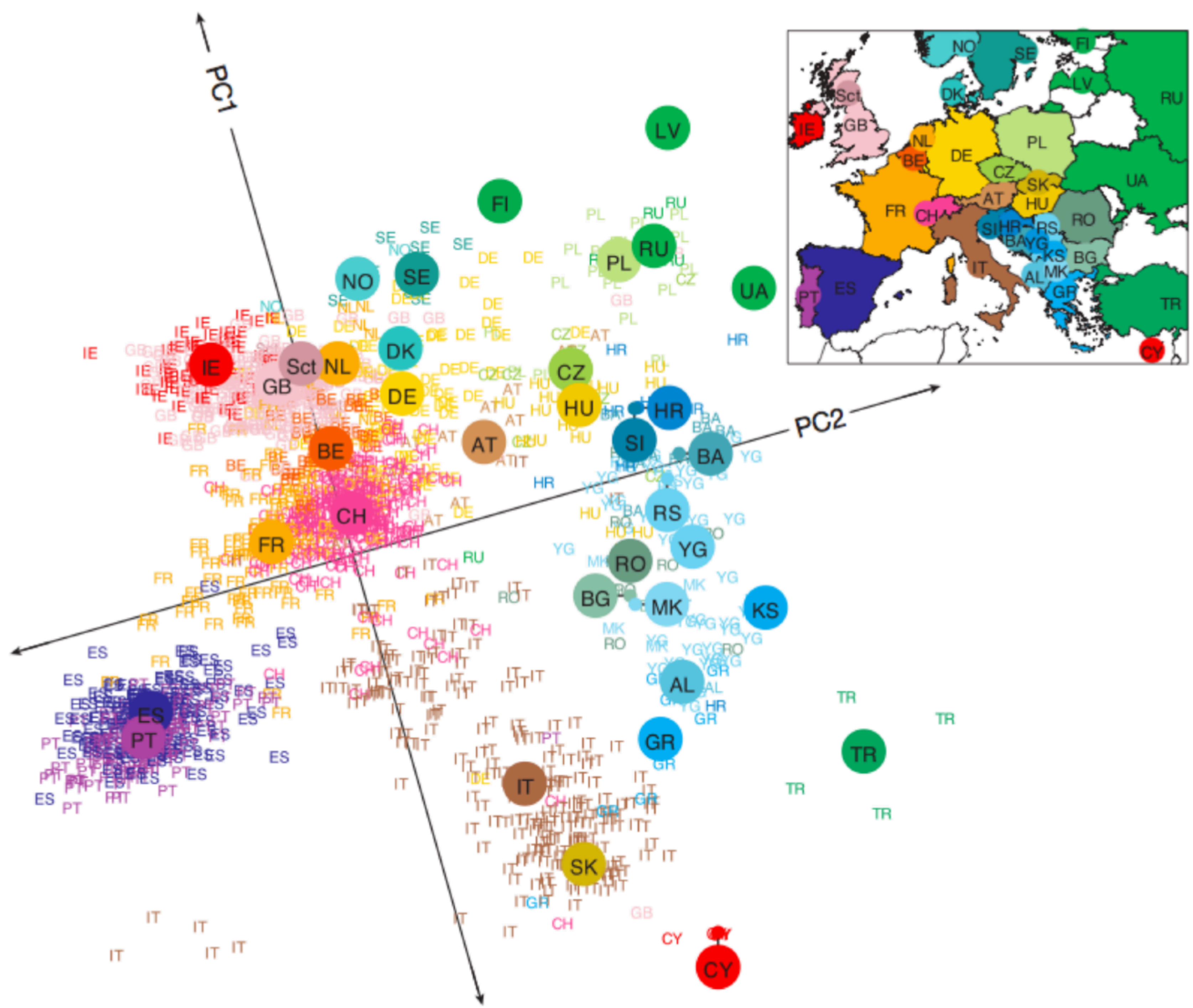
  * If your data has lots of dimensions, PCA finds new dimensions along which the data vary a lot (the long axis of the ellipse)

  * and dimensions along which the data don’t vary much at all, and can be ignored (the short axis)

EXAMPLE: HUMAN GENETICS

* Hundreds of Europeans are genotyped for thousands of genes

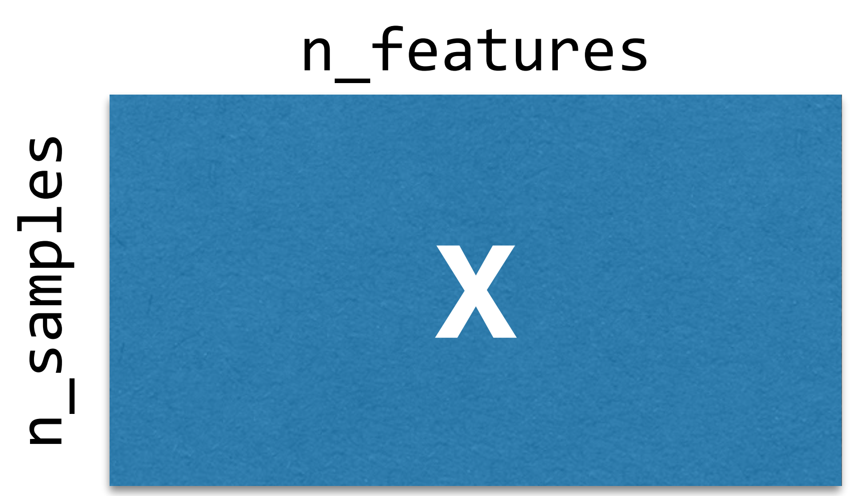
* This info is reduced to 2 dimensions using PCA



HOW DO YOU USE IT

* The input to PCA is a matrix **X** with shape (n_samples, n_features)

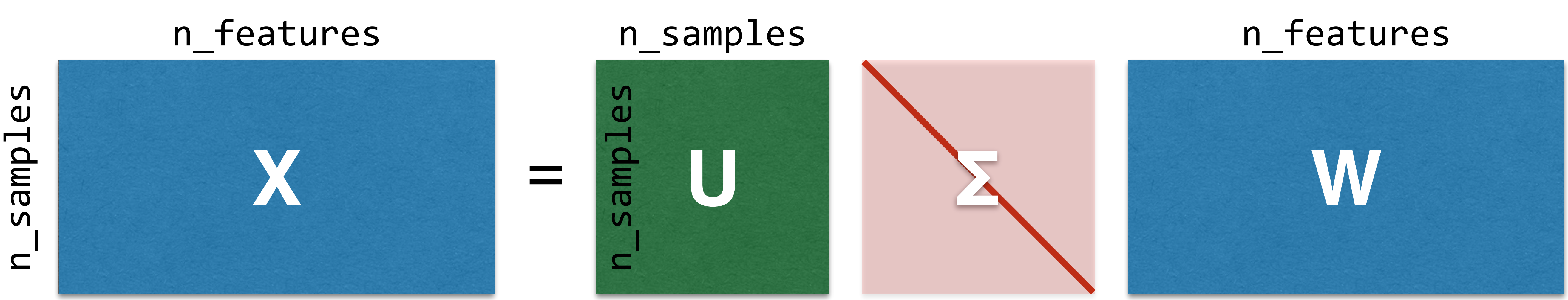
* (Assume that each column of **X** has zero mean. If this isn't true, you can make it true!)



HOW DO YOU USE IT

* PCA represents **X** as a product of 3 matrices: **U**, **Sigma**, and **W**

* (Here assuming that n_features > n_samples)

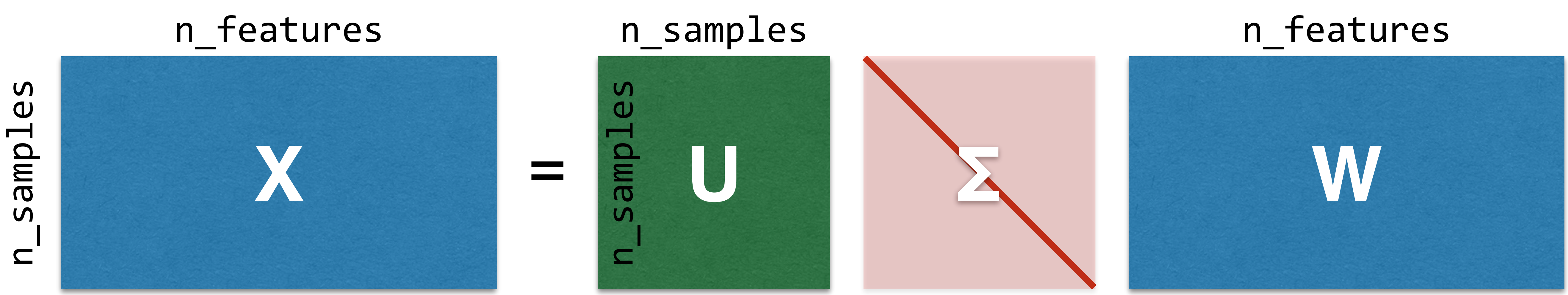


HOW DO YOU USE IT

* **W** contains the **principal components** (each row is one)

* **U** is the **score matrix**, which tells you how much of each PC is in each sample

* **Sigma** is a diagonal matrix of **singular values**, which tell you how "big" (or important) each PC is



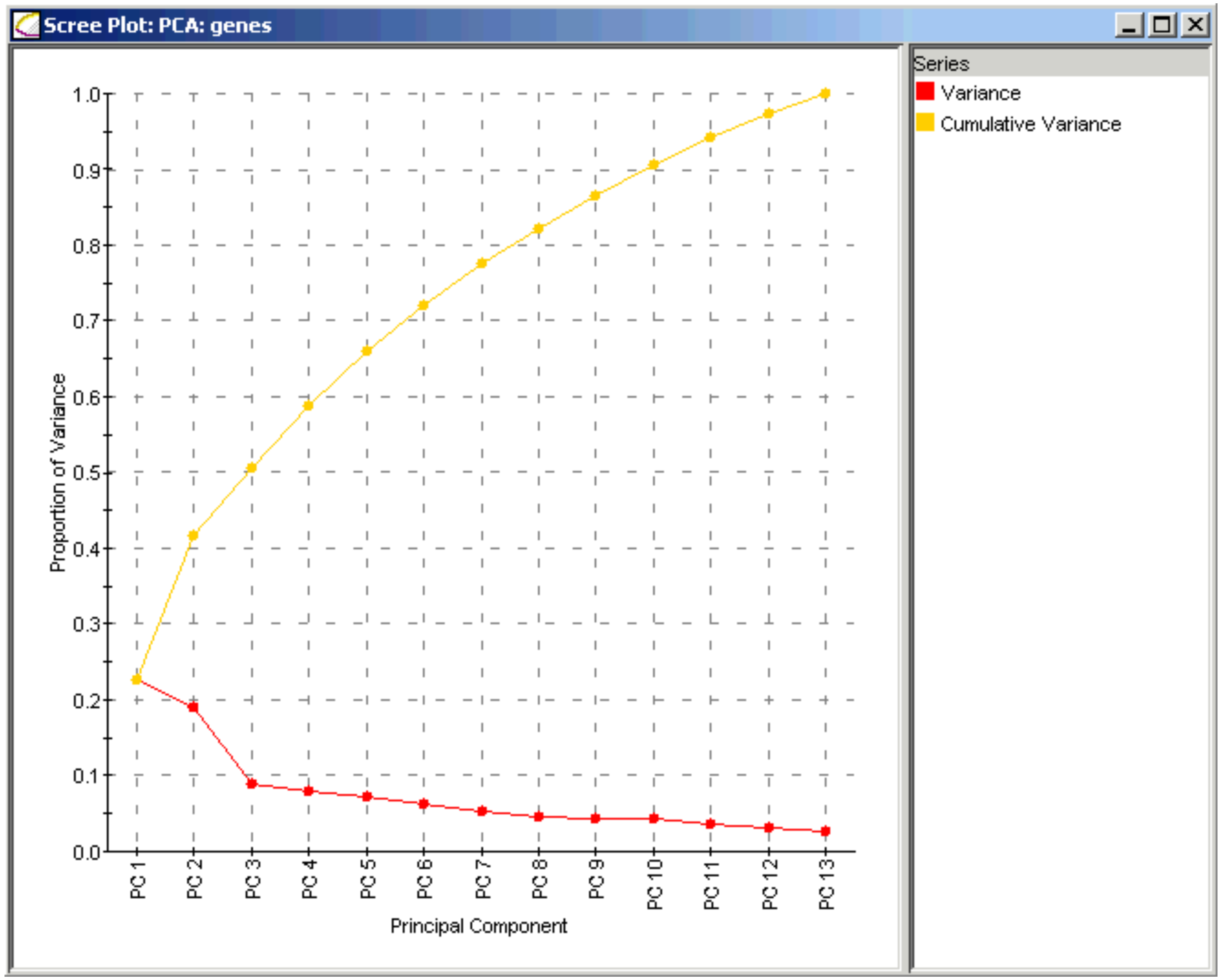
HOW DO YOU USE IT

* You can then visualize the scores (data projected onto PCs), the PCs themselves, and the singular values

HOW DO YOU USE IT

* Singular values are typically visualized as a “Scree plot”

* this shows how much **variance** each component accounts for in the dataset



HOW DO YOU USE IT

* (If you’re familiar with the **singular value decomposition** (SVD), this is exactly the same thing)

* you can use the SVD directly with **np.linalg.svd**

HOW DO YOU USE IT

* But it’s better to do PCA through scikit-learn with **sklearn.decomposition.PCA**

* (This has more options, and will do nice things like subtract the column means for you.)

PCA APPLICATIONS

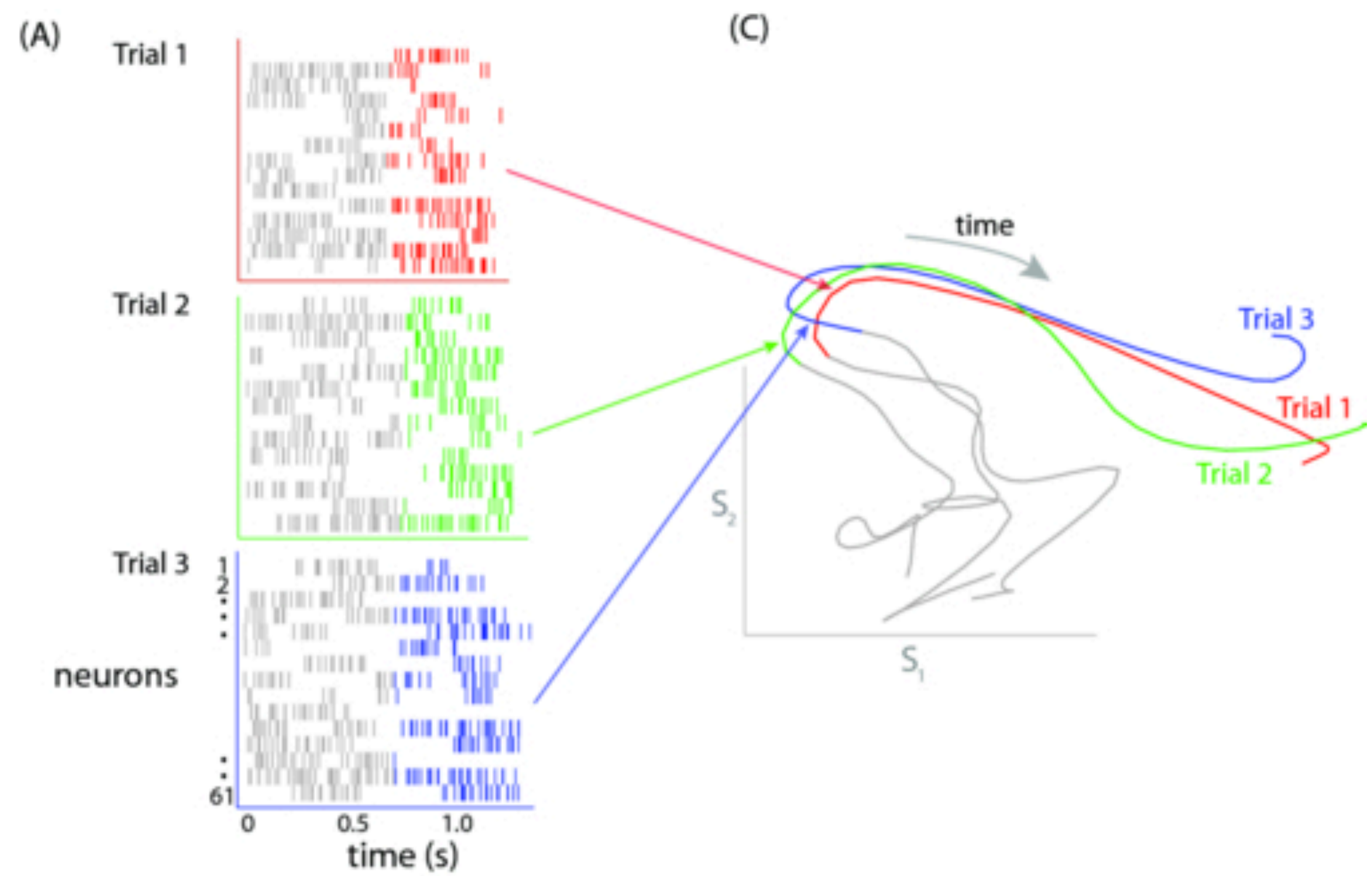
* PCA can be used for either *data analysis* or *data visualization* (and often both)

* It should probably be your #1 go-to visualization tool whenever you have lots of features and don't know how to look at them

PCA APPLICATIONS

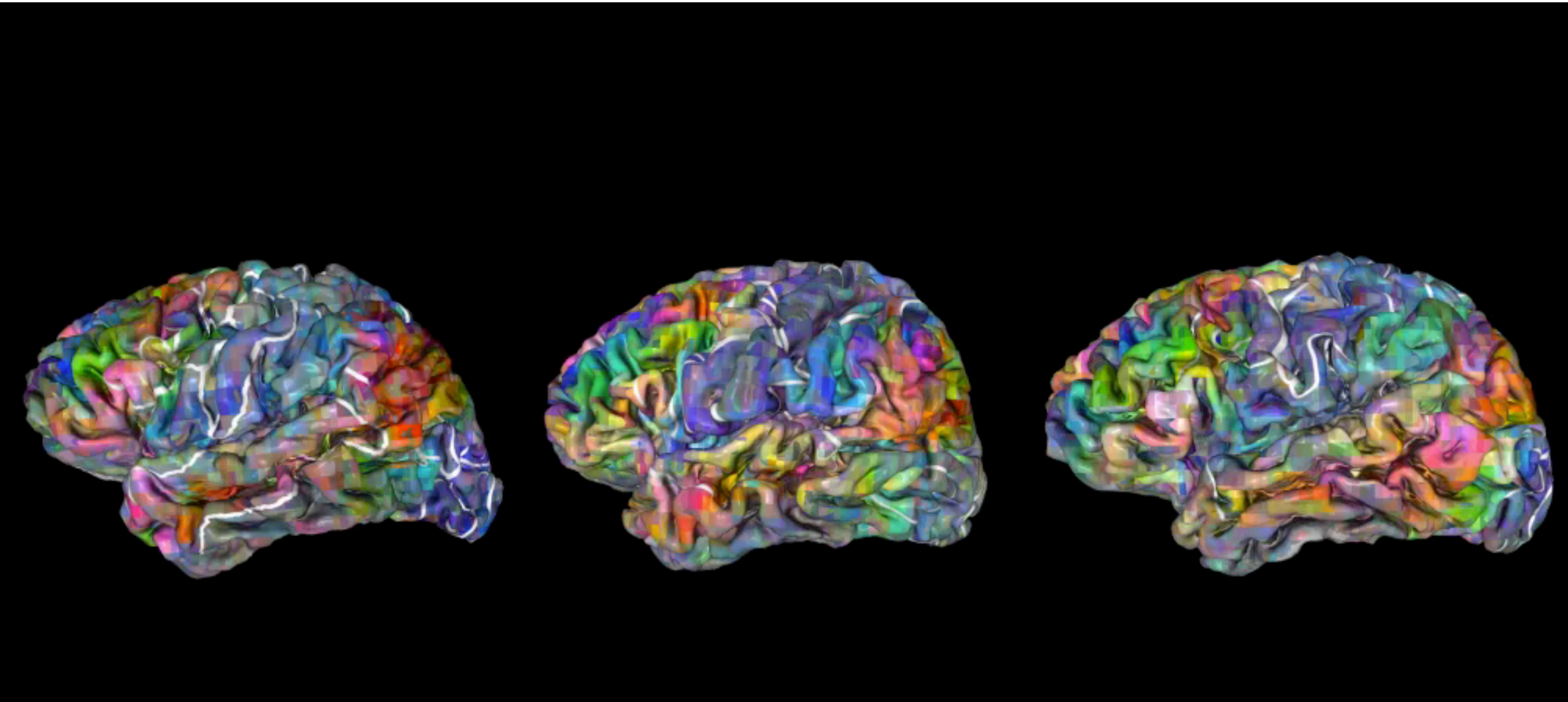
* population analyses of neural activity

* PCA gives a “neural state space”



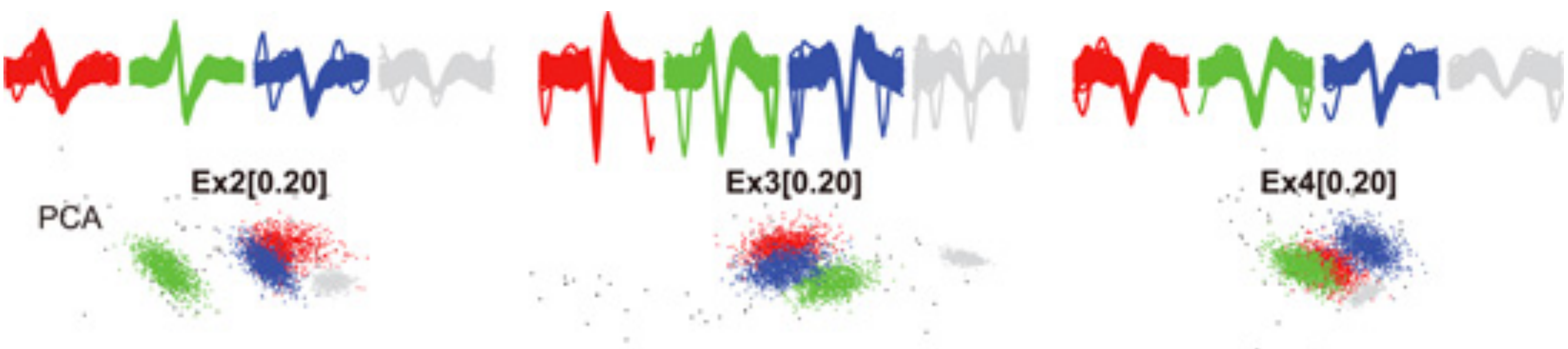
PCA APPLICATIONS

* visualization of high-dimensional regression models



PCA APPLICATIONS

* spike sorting!



PCA APPLICATIONS

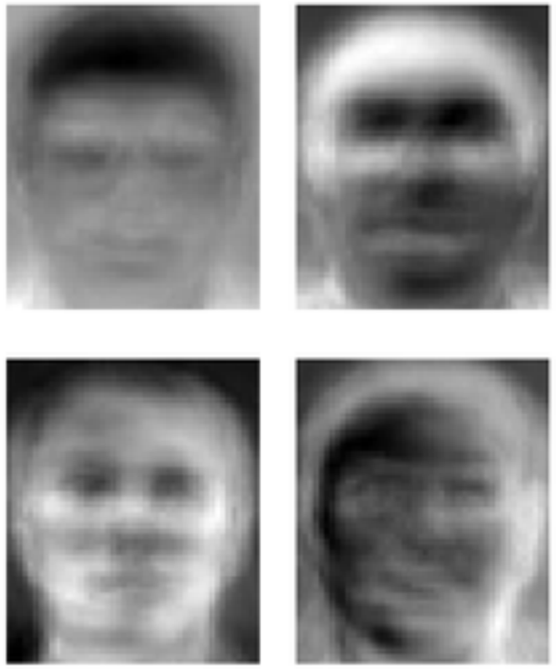
* it's almost certain that PCA is something that *individual neurons do*

* Hebbian learning ("neurons that fire together wire together") results in a neuron learning the **first principal component** of its inputs

PCA APPLICATIONS

* do PCA on a whole bunch of (aligned) face images to get "eigenfaces" – basis functions that all face images are built out of

* it turns out this might fundamental to how individual neurons represent faces! (Chang & Tsao, *Cell* 2017)



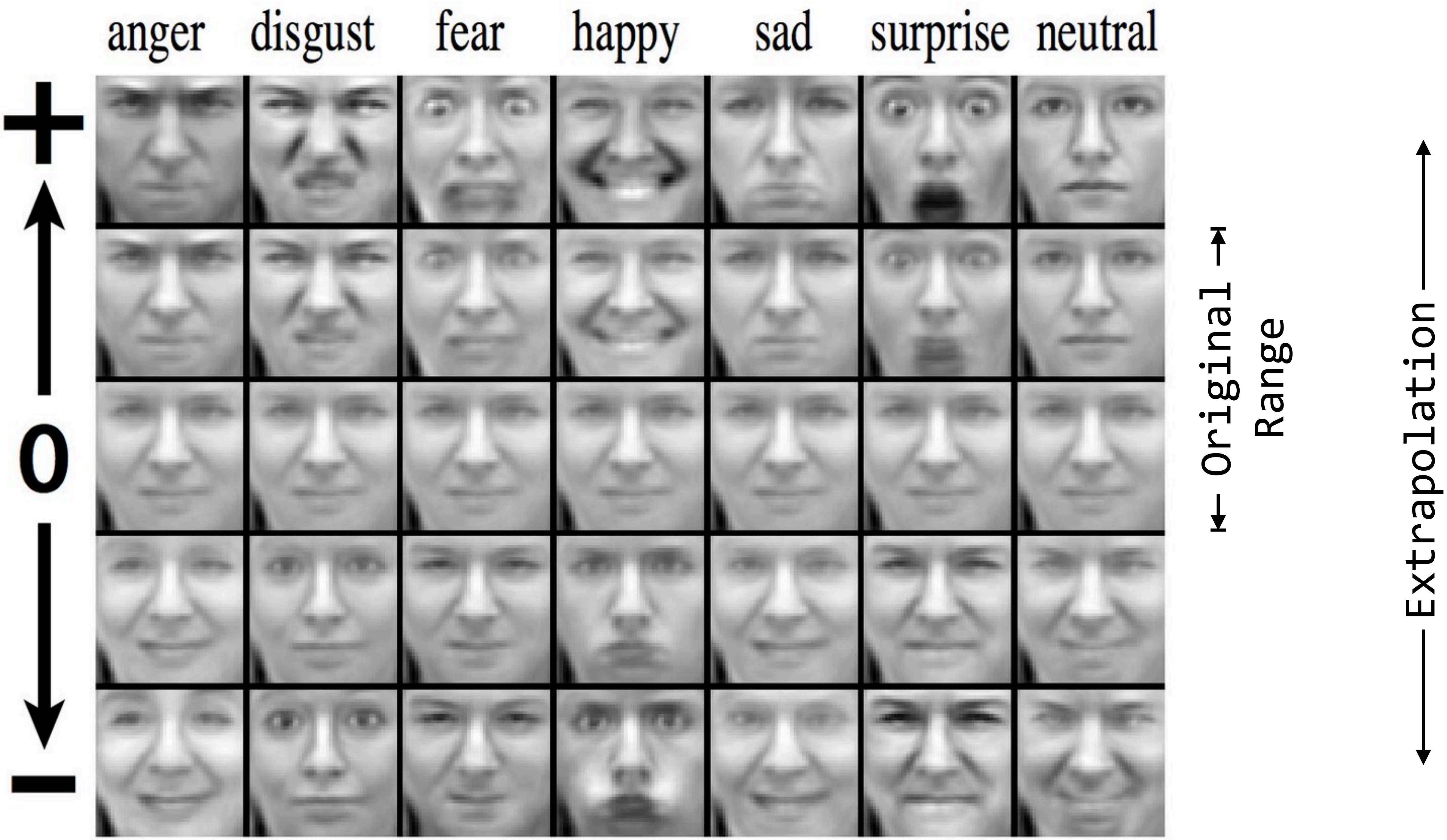
PCA EXTENSIONS: AUTOENCODERS

* autoencoders are artificial neural networks that push each sample through a “bottleneck layer” and then try to reconstruct the original sample

* simple (linear) autoencoders compute exactly PCA

* more complicated ones can do very cool stuff

PCA EXTENSIONS: AUTOENCODERS



from Cheung, Livezey, Bansal, & Olshausen (2015)

MORE RESOURCES

* If you want to learn more about PCA, see this great chapter from PDSH: https://jakevdp.github.io/PythonDataScienceHandbook/05.09-principal-component-analysis.html

THANK YOU!