APS1070

Foundations of Data Analytics and Machine Learning

Winter 2022

Week 7:

- *Projections*
- *Matrix Decompositions*
- *Principal Component Analysis (PCA)*

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Slide Attribution

These slides contain materials from various sources. Special thanks to the following authors:

- Scott Sanner
- Ali Hadi Zadeh
- Jason Riordon

Last Time

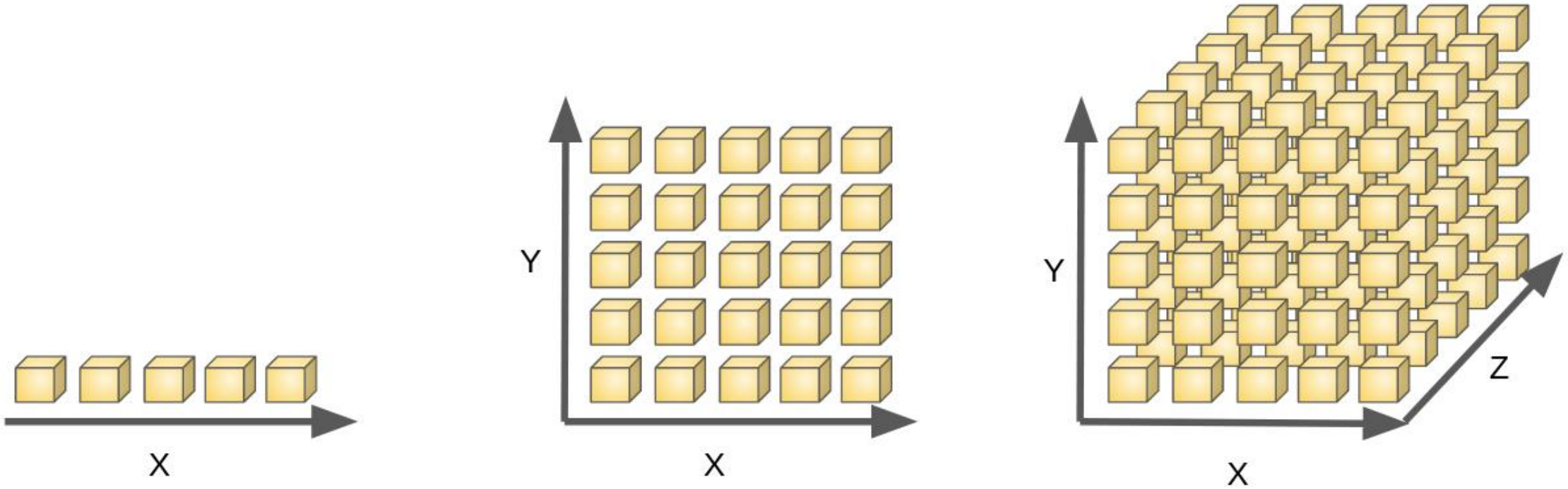
- Looked at linear algebra for data processing in the form of **Data Augmentation**
  - scalars, vectors and matrices
  - solving systems of equations
  - change of basis
  - analytical geometry
  - rotations and other transformations

- Today we will examine data processing in the form of **Dimensionality Reduction**

High-Dimensional Data

- Real world data is often high-dimensional!
- Challenge: difficult to **analyze**, **visualize** and **interpret**

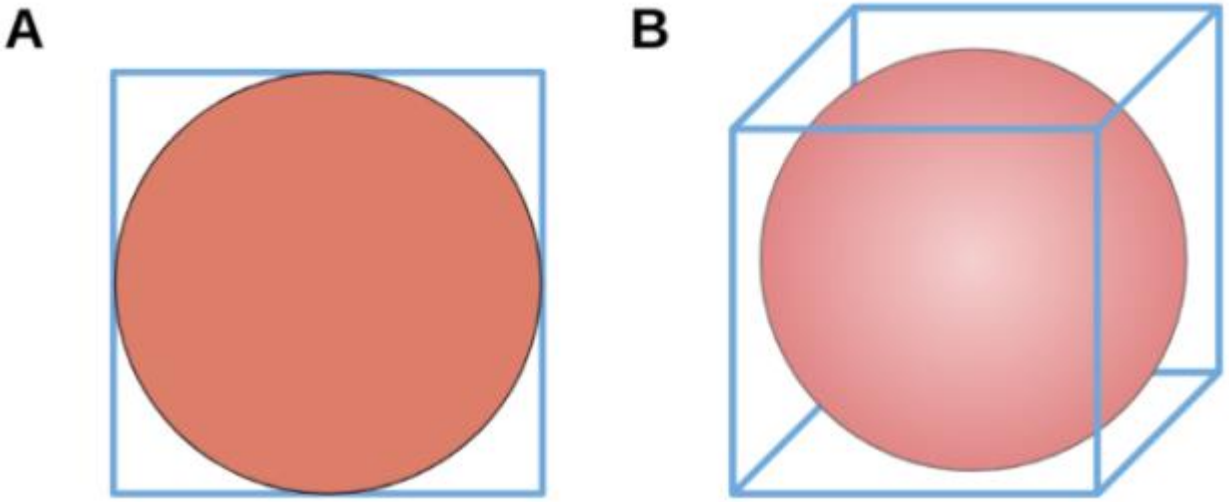
Curse of Dimensionality

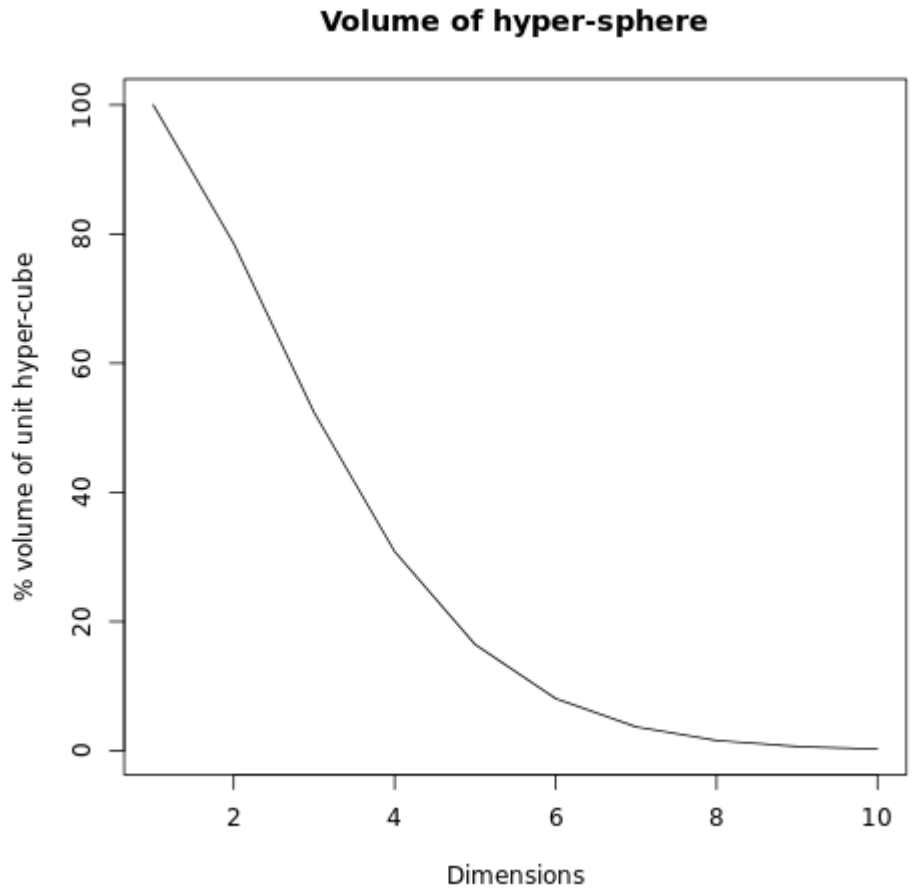


Source: Peter Gleeson

- As the number of feature or dimensions grows, the amount of data we need to generalize accurately grows exponentially.

Curse of Dimensionality





- Majority of the volume is outside of the sphere in higher dimensions

Source: Peter Gleeson

Curse of Dimensionality

- Many dimensions are unnecessary
- Data often lives on a low-dimensional manifold
- Dimensionality reduction finds the relevant dimensions

Agenda

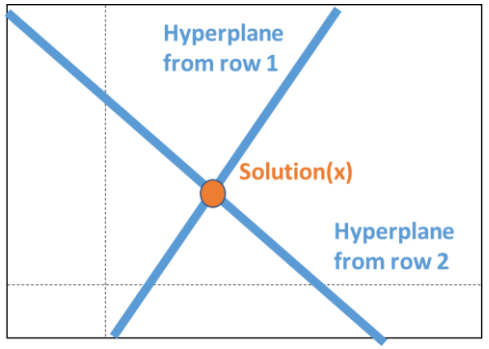
- Projections
- Matrix Decompositions
  - Determinant
  - Trace
  - Eigenvalues and Eigenvectors
  - Eigendecomposition
- PCA
- Dimensionality Reduction

Theme:
Dimensionality Reduction
Part 1

Recap: Linear Algebra

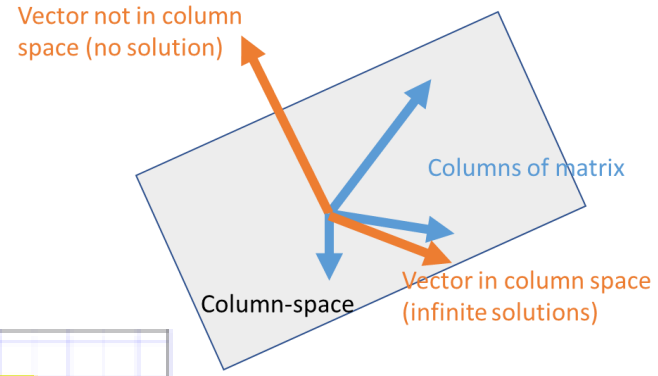
- Given A and b, we want to solve for x:

$$Ax = b \qquad \begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$



- This can be given several interpretations:
  - **By rows**: x is the intersection of hyper-planes:

$$2x - y = 1$$
$$x + y = 5$$

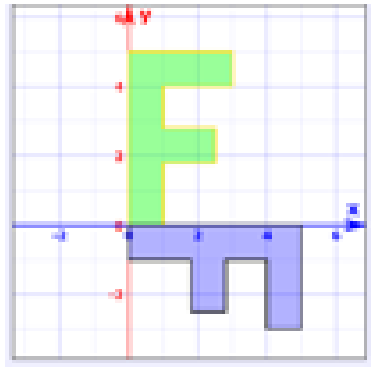


  - **By columns**: x is the linear combination that gives b:

$$x \begin{bmatrix} 2 \\ 1 \end{bmatrix} + y \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$

  - **Transformation**: x is the vector transformed to b:

$$T(x) = b$$



Recap: Analytical Geometry

- Projections are linear transformations that project to lower dimensional feature space

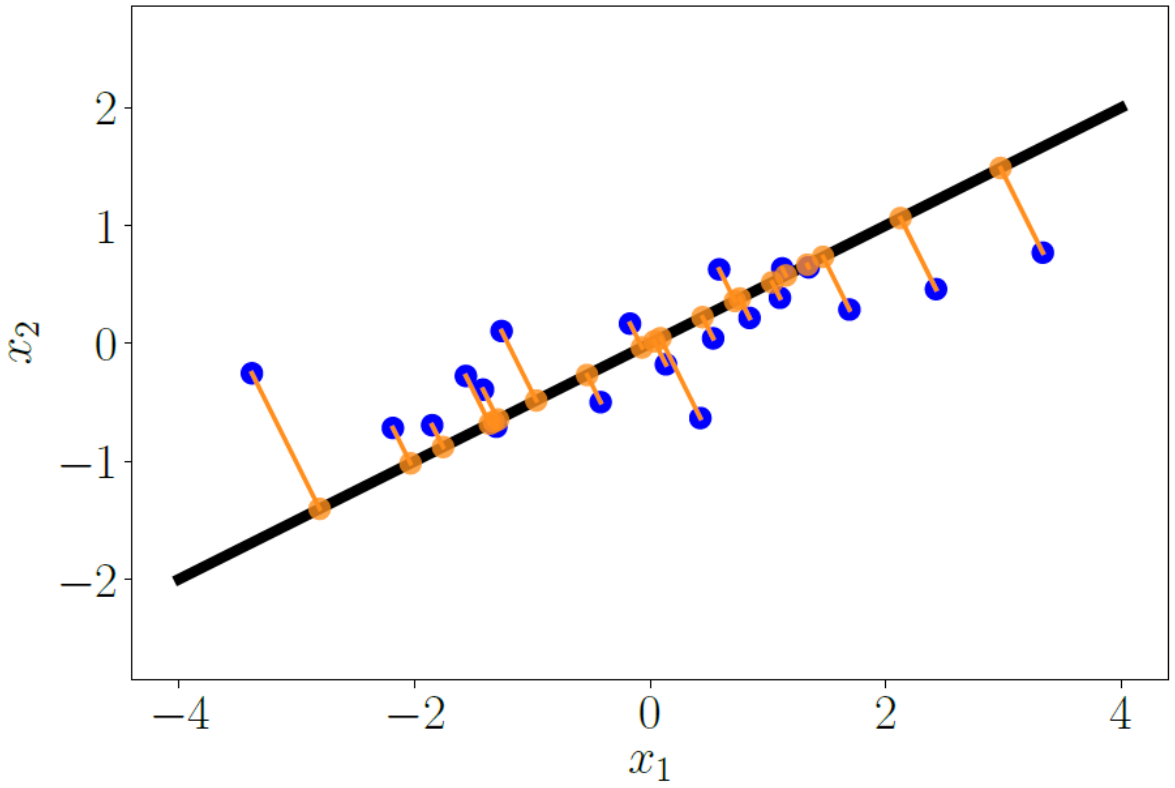
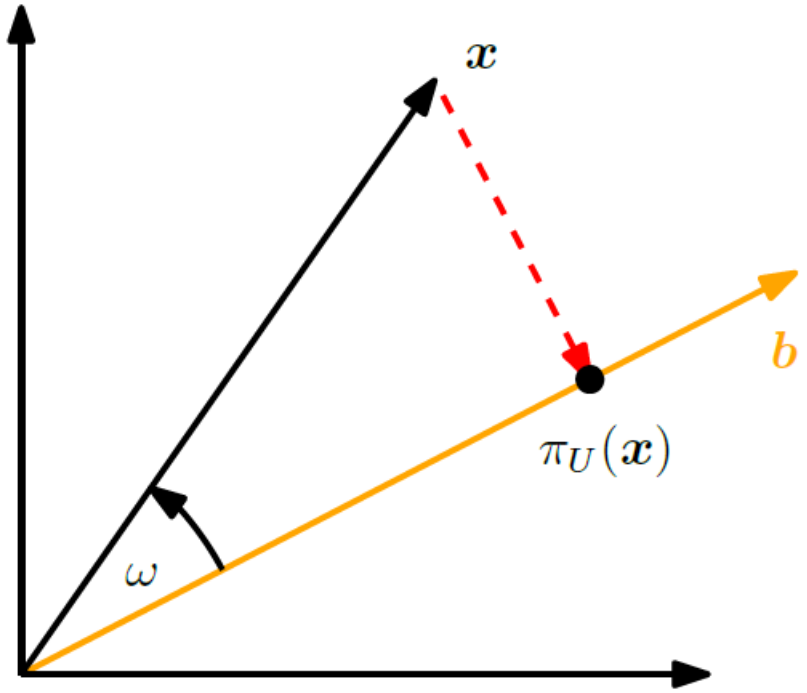


Figure 3.9 Orthogonal projection (orange dots) of a two-dimensional dataset (blue dots) onto a one-dimensional subspace (straight line).

Recap: Orthogonal Projections

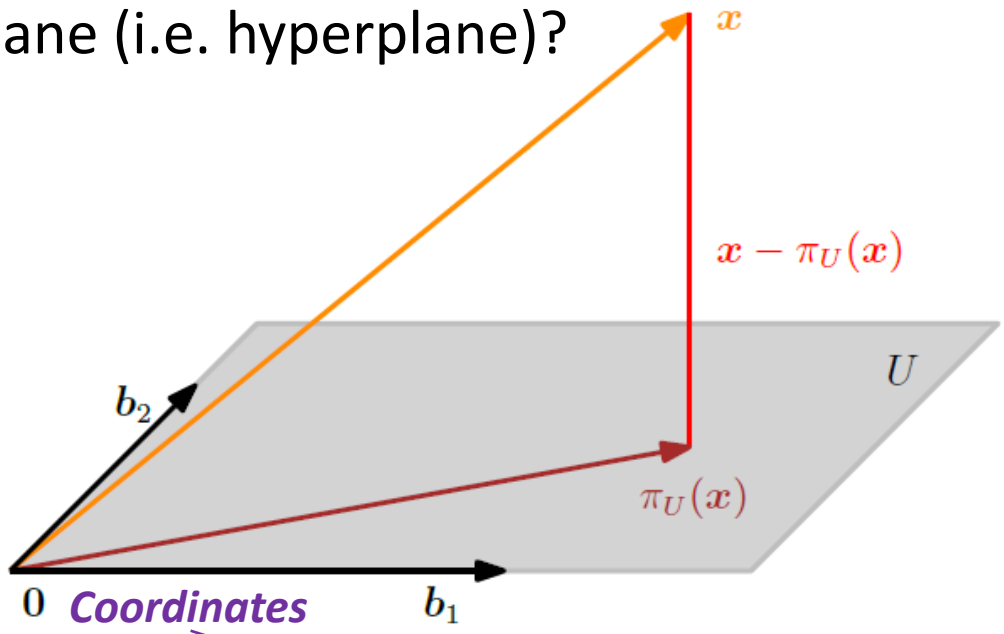
Project vector onto another vector



Coordinate

$$\pi_U(\boldsymbol{x}) = \lambda \boldsymbol{b} = \boldsymbol{b}\frac{\boldsymbol{b}^T\boldsymbol{x}}{\|\boldsymbol{b}\|^2} = \frac{\boldsymbol{b}\boldsymbol{b}^T}{\|\boldsymbol{b}\|^2}\boldsymbol{x}$$

Now let's consider the case of projecting a vector onto a plane (i.e. hyperplane)?

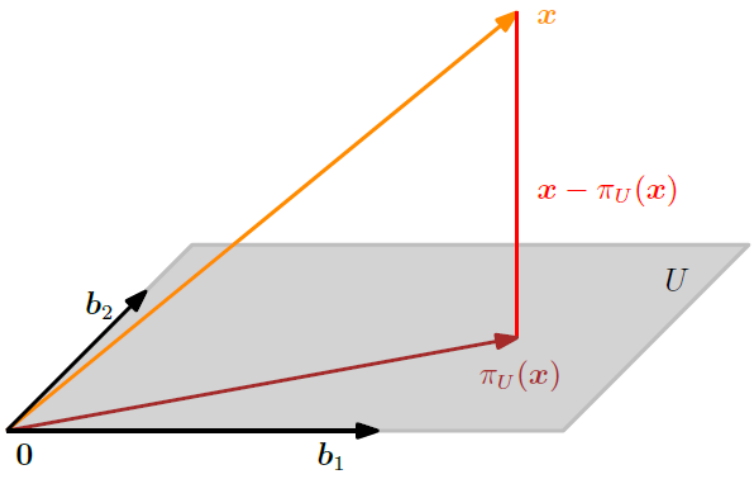


Coordinates

$$\pi_U(\boldsymbol{x}) = \boldsymbol{B}\lambda$$
$$\boldsymbol{B}^T\boldsymbol{B}\lambda = \boldsymbol{B}^T\boldsymbol{x}$$

Example

$$\boldsymbol{B^T B\lambda = B^T x}$$



Example 3.11 (Projection onto a Two-dimensional Subspace)

For a subspace $U = \text{span}[\begin{bmatrix}1\\1\\1\end{bmatrix}, \begin{bmatrix}0\\1\\2\end{bmatrix}] \subseteq \mathbb{R}^3$ and $\boldsymbol{x} = \begin{bmatrix}6\\0\\0\end{bmatrix} \in \mathbb{R}^3$ find the coordinates $\boldsymbol{\lambda}$ of $\boldsymbol{x}$ in terms of the subspace U, the projection point $\pi_U(\boldsymbol{x})$ and the projection matrix $\boldsymbol{P}_\pi$.

First, we see that the generating set of U is a basis (linear independence) and write the basis vectors of U into a matrix $\boldsymbol{B} = \begin{bmatrix}1 & 0\\1 & 1\\1 & 2\end{bmatrix}$.

Second, we compute the matrix $\boldsymbol{B}^\top\boldsymbol{B}$ and the vector $\boldsymbol{B}^\top\boldsymbol{x}$ as

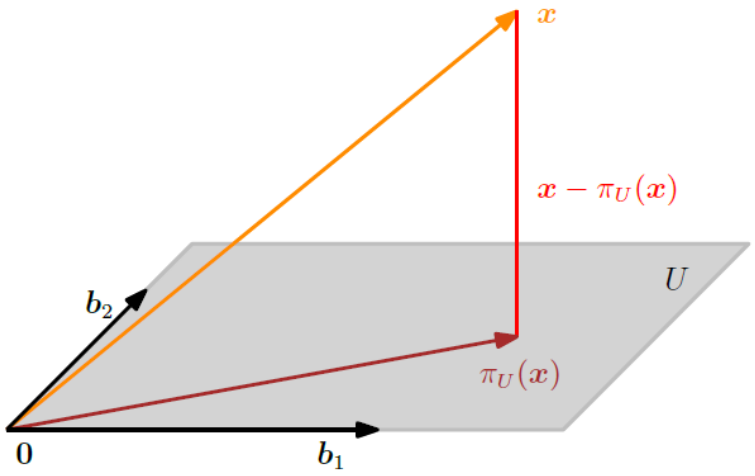
$$\boldsymbol{B}^\top\boldsymbol{B} = \begin{bmatrix}1 & 1 & 1\\0 & 1 & 2\end{bmatrix}\begin{bmatrix}1 & 0\\1 & 1\\1 & 2\end{bmatrix} = \begin{bmatrix}3 & 3\\3 & 5\end{bmatrix}, \quad \boldsymbol{B}^\top\boldsymbol{x} = \begin{bmatrix}1 & 1 & 1\\0 & 1 & 2\end{bmatrix}\begin{bmatrix}6\\0\\0\end{bmatrix} = \begin{bmatrix}6\\0\end{bmatrix}. \tag{3.60}$$

Third, we solve the normal equation $\boldsymbol{B}^\top\boldsymbol{B}\boldsymbol{\lambda} = \boldsymbol{B}^\top\boldsymbol{x}$ to find $\boldsymbol{\lambda}$:

$$\begin{bmatrix}3 & 3\\3 & 5\end{bmatrix}\begin{bmatrix}\lambda_1\\\lambda_2\end{bmatrix} = \begin{bmatrix}6\\0\end{bmatrix} \iff \boldsymbol{\lambda} = \begin{bmatrix}5\\-3\end{bmatrix}. \tag{3.61}$$

Example con't

$$B\lambda = B\left(B^T B\right)^{-1} B^T x$$



Third, we solve the normal equation $B^\top B\boldsymbol{\lambda} = B^\top \boldsymbol{x}$ to find $\boldsymbol{\lambda}$:

$$\begin{bmatrix} 3 & 3 \\ 3 & 5 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 0 \end{bmatrix} \iff \boldsymbol{\lambda} = \begin{bmatrix} 5 \\ -3 \end{bmatrix}. \tag{3.61}$$

Fourth, the projection $\pi_U(\boldsymbol{x})$ of $\boldsymbol{x}$ onto U, i.e., into the column space of B, can be directly computed via

$$\pi_U(\boldsymbol{x}) = B\boldsymbol{\lambda} = \begin{bmatrix} 5 \\ 2 \\ -1 \end{bmatrix}. \tag{3.62}$$

The corresponding *projection error* is the norm of the difference vector between the original vector and its projection onto U, i.e.,

$$\|\boldsymbol{x} - \pi_U(\boldsymbol{x})\| = \left\| \begin{bmatrix} 1 & -2 & 1 \end{bmatrix}^\top \right\| = \sqrt{6}. \tag{3.63}$$

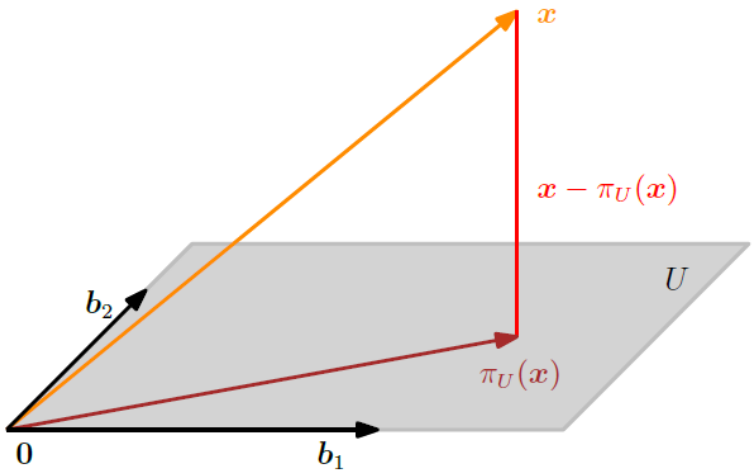
Fifth, the projection matrix (for any $\boldsymbol{x} \in \mathbb{R}^3$) is given by

$$P_\pi = B(B^\top B)^{-1} B^\top = \frac{1}{6} \begin{bmatrix} 5 & 2 & -1 \\ 2 & 2 & 2 \\ -1 & 2 & 5 \end{bmatrix}. \tag{3.64}$$

To verify the results, we can (a) check whether the displacement vector $\pi_U(\boldsymbol{x}) - \boldsymbol{x}$ is orthogonal to all basis vectors of U, and (b) verify that $P_\pi = P_\pi^2$ (see Definition 3.10).

Projection onto a subspace with orthonormal bases

$$B\lambda = B\left(B^T B\right)^{-1} B^T x$$



If we have orthonormal bases (B), then this simplifies the calculation of the inverse because $B^T = B^{-1}$

$$B\lambda = BB^T x$$

Google Colab Code

“how to summarize matrices, how matrices can be decomposed, and how these decompositions can be used for matrix approximations”

Matrix Decompositions

Readings:

- **Chapter 4.1-5 MML Textbook**

Decomposing a Matrix - 1

- There are many ways we can describe a matrix
- Example, take a look at the following transformation:

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 5 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

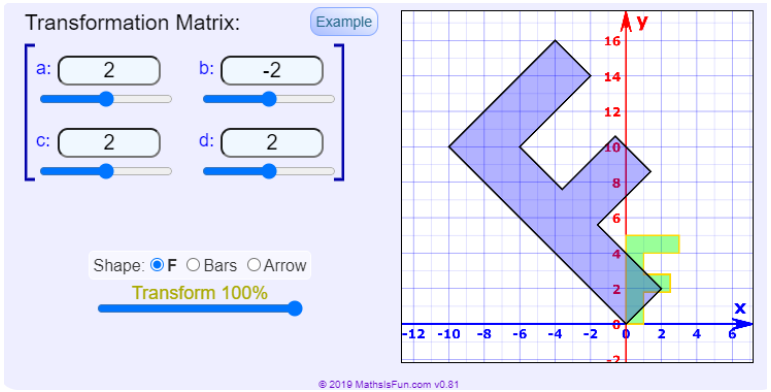
- Notice that we could write the same thing in terms of several transformations:

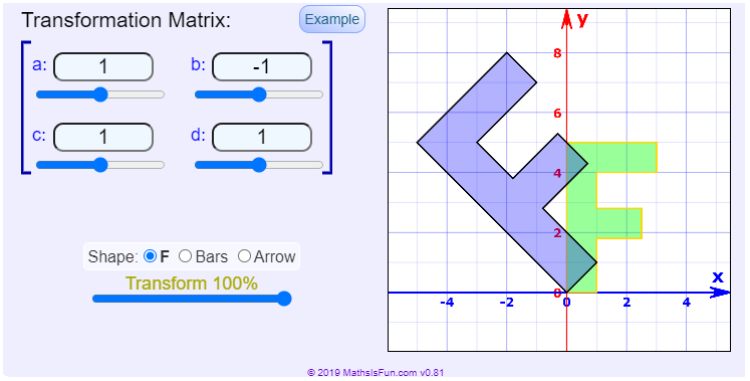
$$A = \begin{bmatrix} 1 & 0 & 0 \\ 5 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 5 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

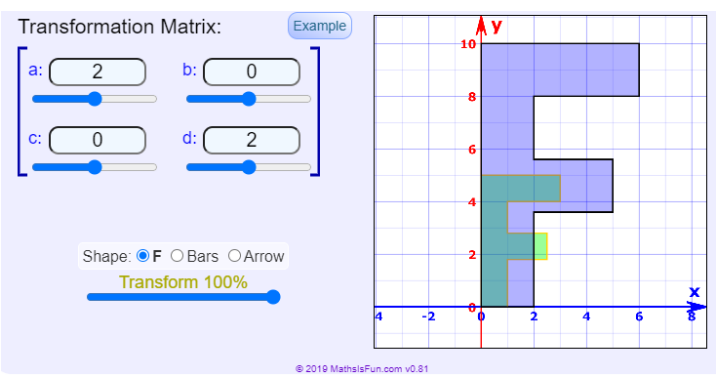
Decomposing a Matrix - 2

- There are many ways we can describe a matrix
- Example, take a look at the following transformation $A = \begin{bmatrix} 2 & -2 \\ 2 & 2 \end{bmatrix}$
- Notice that we could write the same thing in terms of several transformations:

$$A = \begin{bmatrix} 2 & -2 \\ 2 & 2 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$







Decomposing a Matrix

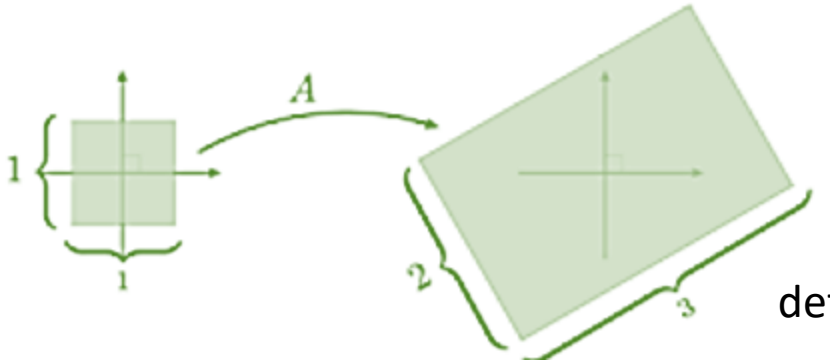
- This can be used for providing clarity on what the transformation is doing
- Simplifying and speeding up computations
- Dimensionality reduction as we'll see later

Key Concepts

- Determinant
- Trace
- Diagonalization
- Eigenvectors
- Eigenvalues

Determinant

- The determinant of a square matrix is a function that maps A onto a real number.
- Simple geometric meaning.
  - calculates how volume grows/shrinks under a linear transformation/mapping
  - for example:



det(A) = 6

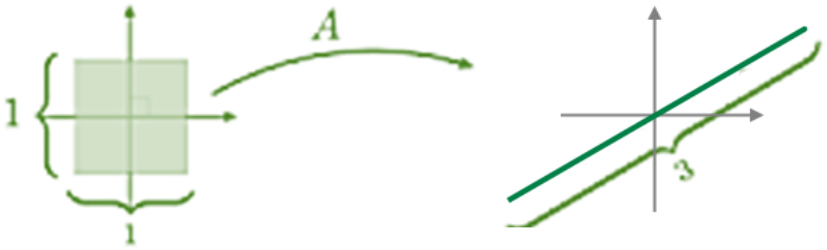
$$\det(\boldsymbol{A}) = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix}$$

Two vertical bars indicate determinant of matrix enclosed inside

Determinant for Matrix Invertibility

- What does it mean when a matrix is not invertible?

- Simple geometric meaning.
  - transformation to a subspace
  - how does the volume grows/shrinks?
  - for example:



det(A) = 0

Note:

If det(A) = 0, then matrix A is singular.

Determining the Determinant

- The determinant can only be calculated on square matrices (n x n):

- Determinant in 2d:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

- Determinant in 3d:

recursively take alternating sums of sub-determinants

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = a_{11}\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} - a_{12}\begin{bmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{bmatrix} + a_{13}\begin{bmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}$$

$$= a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23} - a_{31}a_{22}a_{13} - a_{11}a_{32}a_{23} - a_{21}a_{12}a_{33}$$

Determining the Determinant

- Can you think of an easier way?

- Hint: what is the determinant of the following upper triangular matrix?

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{bmatrix}$$

$$\det(A) = a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23} - a_{31}a_{22}a_{13} - a_{11}a_{32}a_{23} - a_{21}a_{12}a_{33}$$

$$= a_{11}a_{22}a_{33}$$

- Q: How can we obtain a triangular matrix?

Determining the Determinant

- Apply Gaussian Elimination to bring matrix into row Echelon form.
- Then determinant comes directly from the diagonal:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{bmatrix} \leftarrow \det(A) = \prod_{i}^{n} a_{ii}$$

for triangular matrix

- There are three things to consider:
  1. Row addition has no effect on determinant
  2. Each row switching operation changes sign of determinant
  3. Scaling a row scales the determinant

Trace

- The trace of a square matrix is the sum of the diagonal elements.
- It is defined as:

$$\mathbf{tr}(\mathrm{A}) = \sum_{i=1}^{n} a_{ii}$$

$$\mathrm{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

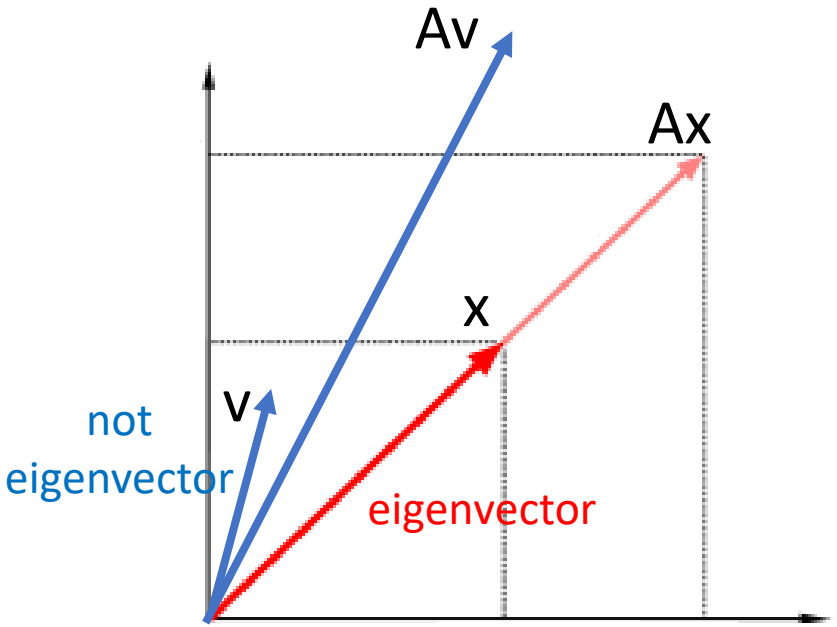
- Has some interesting identities that can help simplify equations:
  - $\mathbf{tr}(c\mathrm{A} + d\mathrm{B}) = c\mathbf{tr}(\mathrm{A}) + d\mathbf{tr}(\mathrm{B})$
  - $\mathbf{tr}(\mathrm{A}^{\mathrm{T}}\mathrm{B}) = \mathbf{tr}(\mathrm{A}\mathrm{B}^{\mathrm{T}}) = \mathbf{tr}(\mathrm{B}^{\mathrm{T}}\mathrm{A})$
  - $\mathbf{tr}(\mathrm{ABC}) = \mathbf{tr}(\mathrm{ACB}) = \mathbf{tr}(\mathrm{BCA})$

Assuming that the dimensions work

Eigenvectors

- Vectors that don't change their direction due to a transformation and can be represented as follows:

$$Ax = \lambda x$$



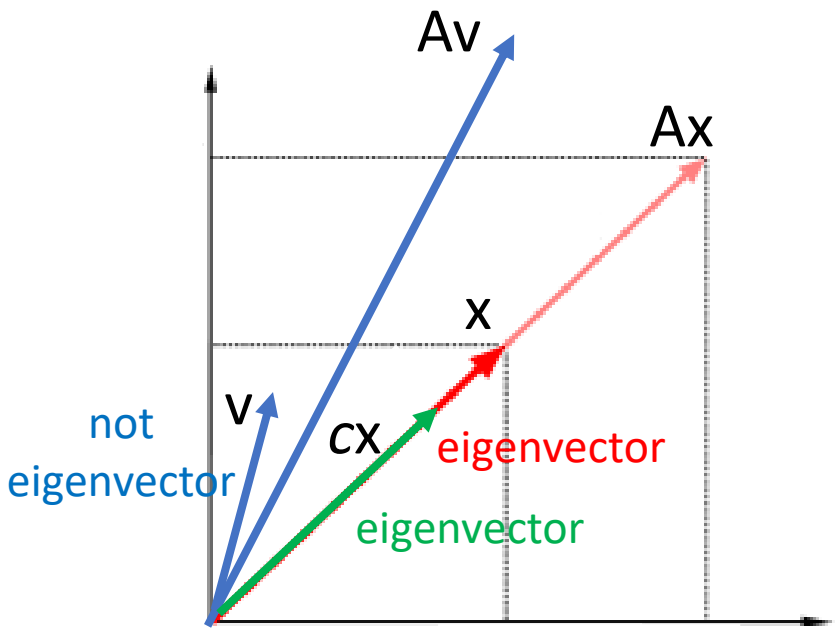
- Depending on the dimension there may be multiple independent vectors that satisfy the equation (eigenvectors).
- Where λ is a scalar referred to as eigenvalue.

Non-Uniqueness of Eigenvectors

- If x is an eigenvector of A with corresponding eigenvalue λ then it holds that *c*x is also an eigenvector of A:

$$A(cx) = cAx = c\lambda x = \lambda(cx)$$

- All vectors that are collinear to x are also eigenvectors of A with the same eigenvalue λ



Finding Eigenvectors

- We can find the characteristic polynomial to find eigenvalues:

$$p_A(\lambda) = \mathbf{det}(\mathrm{A} - \lambda \mathrm{I})$$

$$= \det \begin{bmatrix} a_{11} - \lambda & a_{12} & a_{13} \\ a_{21} & a_{22} - \lambda & a_{23} \\ a_{31} & a_{32} & a_{33} - \lambda \end{bmatrix}$$

$$= c_0\lambda + c_1\lambda^2 + \cdots + c_{n-1}\lambda^{n-1} + -1^n\lambda^n$$

We can describe a matrix A as a polynomial

Aside:

$$\mathrm{Ax} = \lambda \mathrm{x}$$
$$\mathrm{Ax} - \lambda \mathrm{x} = 0$$
$$(\mathrm{A} - \lambda \mathrm{I})\mathrm{x} = 0$$

solve for roots of the polynomial to obtain eigenvalues and eigenvectors!

Theorems

- There are a few theorems worth mentioning:
  1. λ_i is an eigenvalue if and only if λ_i is a root of a characteristic polynomial.
  2. eigenvectors of a square matrix (n x n) with **n distinct eigenvalues** are linearly independent and form a basis of R^n.

Theorems

3. The determinant of a square matrix (n x n) is the product of its eigenvalues.

$$\mathrm{p} = \mathbf{det}(\mathrm{A}) = \prod_{i}^{n} \lambda_i$$

4. The mean of the eigenvalues is the mean of the diagonal entries

i.e. the sum of the eigenvalues is the sum of the diagonal entries

$$\mathrm{m} = \mathbf{tr}(\mathrm{A})/n = \sum_{i=1}^{n} \lambda_i \ /n$$

i.e. the trace of an n x n matrix is the sum of its eigenvalues.

For 2x2 matrices, the eigenvalues are $\lambda_1, \lambda_2 = m \pm \sqrt{m^2 - p}$

Example 4.5

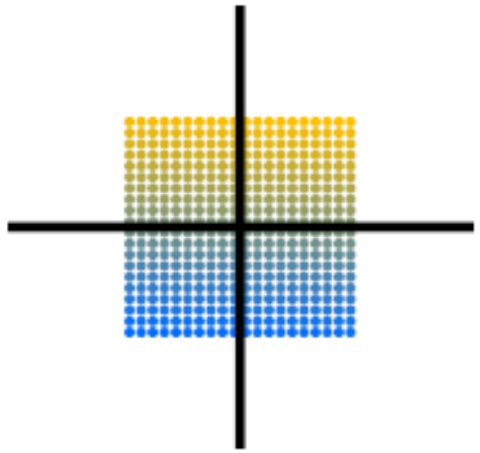
$$\boldsymbol{A} = \begin{bmatrix} 4 & 2 \\ 1 & 3 \end{bmatrix}$$

Eigenvalues?
Eigenvectors?

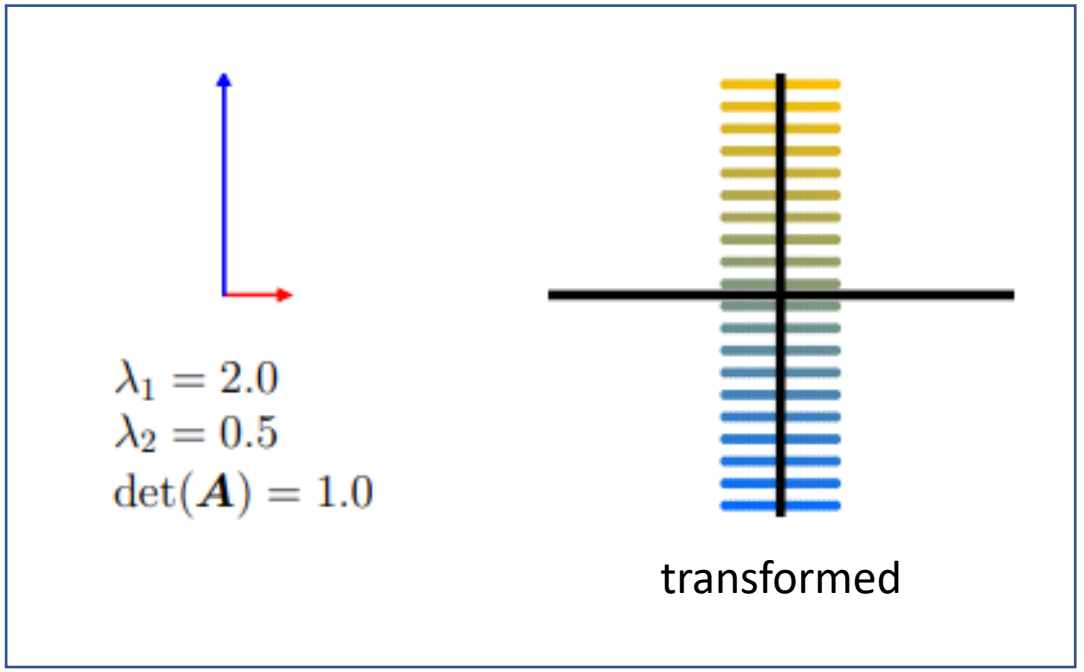
Two numbers with a sum of 7 and a product of 10?

Graphical Intuition - Scaling

$$A = \begin{bmatrix} 1/2 & 0 \\ 0 & 2 \end{bmatrix}$$



original

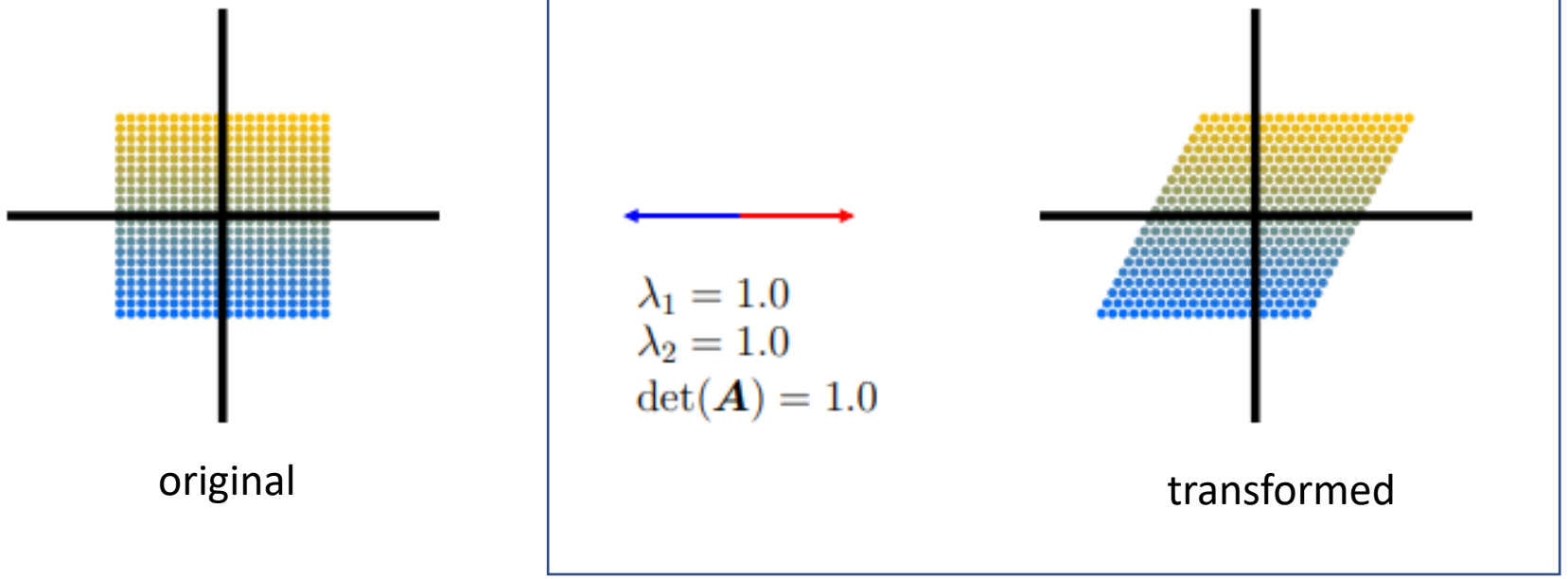


transformed

- The vertical axis stretched by a factor of 2 and the horizontal axis is compressed by a factor of 1/2. The mapping is area preserving.

Graphical Intuition - Shear

$$A = \begin{bmatrix} 1 & 1/2 \\ 0 & 1 \end{bmatrix}$$



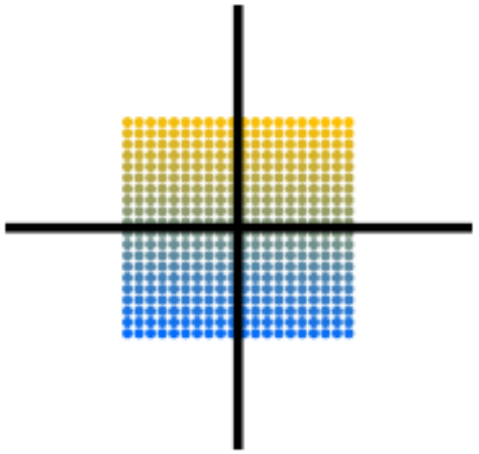
original

transformed

- Sheers the points along the horizontal axis to the right if on positive side of the vertical axis and left if on negative side. Area preserving.

Graphical Intuition - Rotation

$$A = \begin{bmatrix} \cos(\pi/6) & -\sin(\pi/6) \\ \sin(\pi/6) & \cos(\pi/6) \end{bmatrix} = 0.5 \begin{bmatrix} \sqrt{3} & -1 \\ 1 & \sqrt{3} \end{bmatrix}$$



original

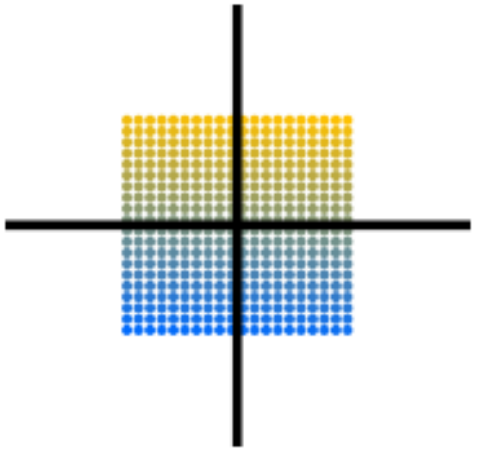
$\lambda_1 = (0.87\text{-}0.5\text{j})$
$\lambda_2 = (0.87\text{+}0.5\text{j})$
$\det(\boldsymbol{A}) = 1.0$

transformed

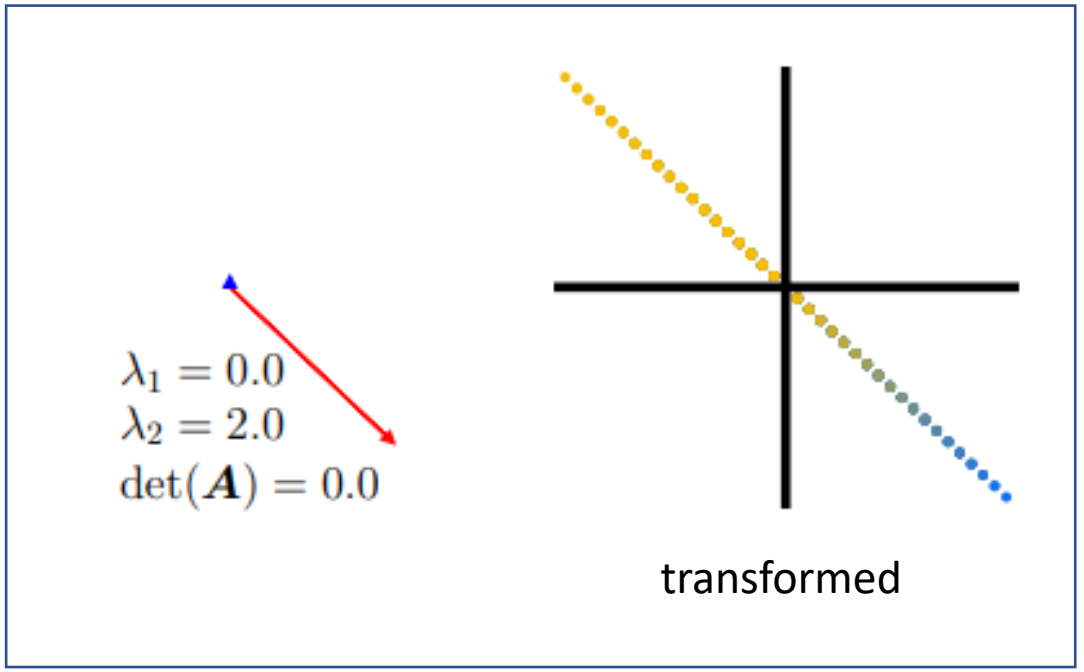
- The matrix rotates the points by $\pi/6$ rad (30 degrees) counterclockwise. The eigenvalues are complex, so cannot draw eigenvectors on real axis. The rotation is area preserving.

Graphical Intuition – Collapse to Subspace

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



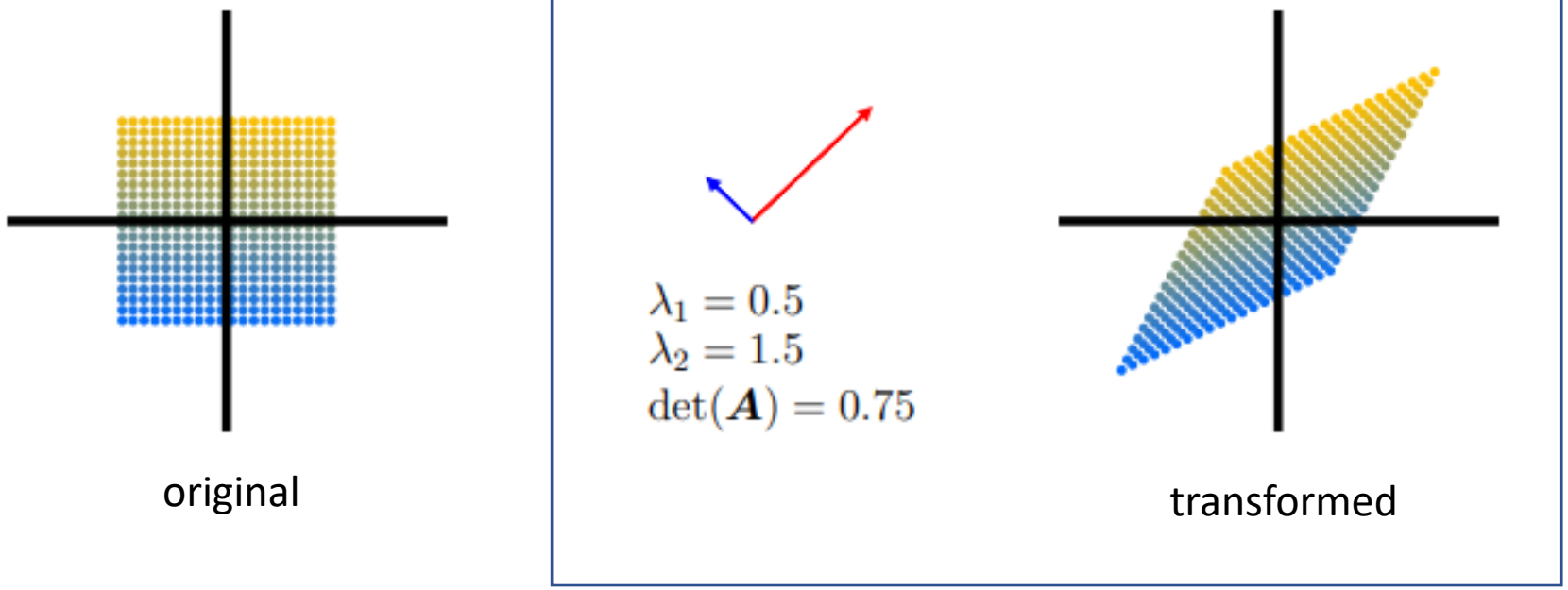
original



- Represents a mapping that collapses a two-dimensional domain onto one dimension. The eigenvalue $\lambda_1 = 0$ collapses while the other stretches the space by 2. The area in this case is 0.

Graphical Intuition – Sheer and Stretch

$$A = \begin{bmatrix} 1 & 1/2 \\ 1/2 & 1 \end{bmatrix}$$



- Represents a shear and stretch mapping. It stretches along the red eigenvector by 1.5 and compresses along blue eigenvector by 0.5. That area is scaled by 75%.

Eigendecomposition

- A **square matrix** (n x n) can be factored into:

$$A = PDP^{-1}$$

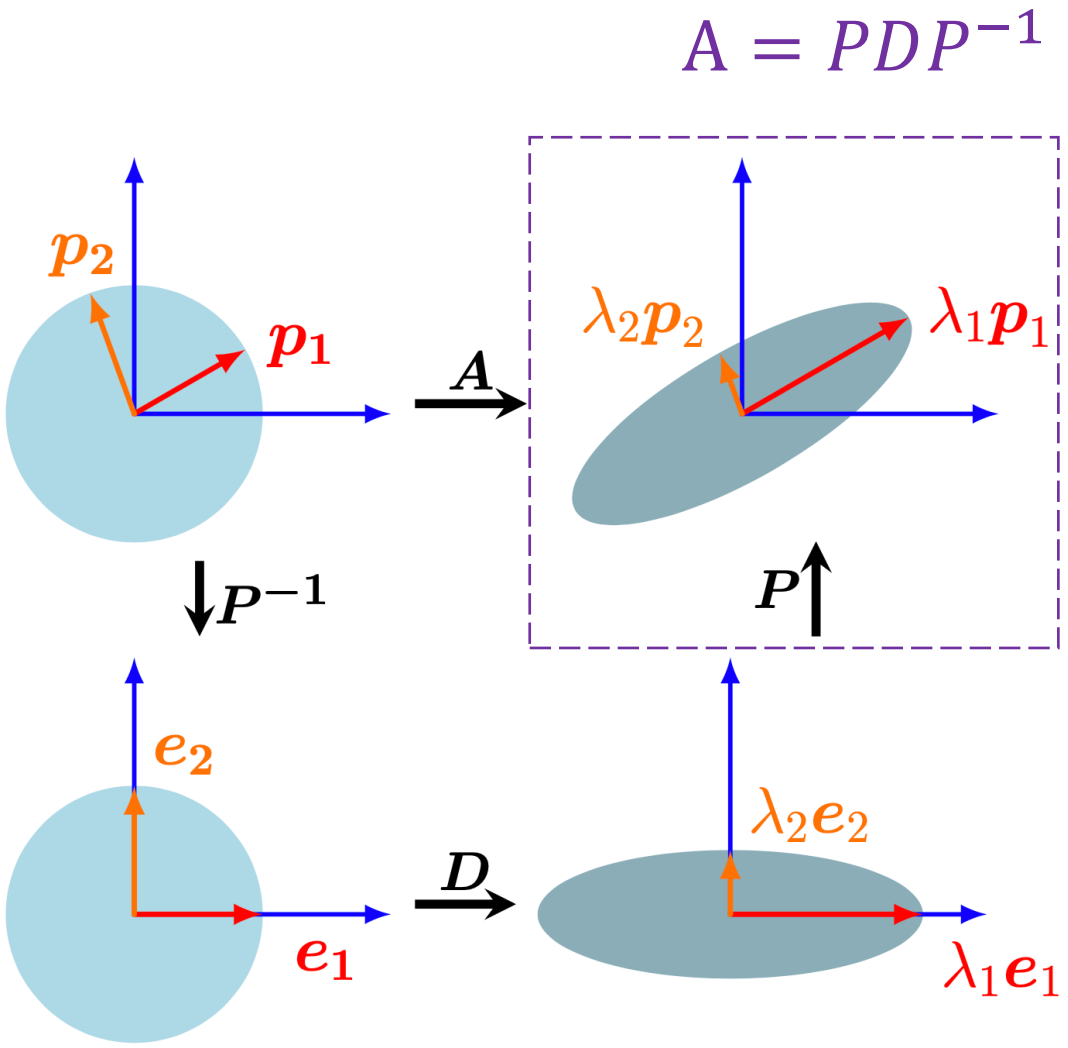
where P is R^{nxn} and D is a diagonal matrix whose diagonal entries are eigenvalues of A (if and only if the eigenvectors form the basis of R^n)

- A **square symmetric matrix** (n x n) the eigenvectors form an orthonormal basis (with real eigenvalues) and A can be factored into:

$$A = PDP^{T}$$ Spectral Theorem

Geometric Intuition

- **Eigendecomposition** can be though of as a sequence of transformations:
  1. **P**$^{-1}$ performs a basis change depicted as a **rotation-like operation** from standard basis into the eigenbasis
  2. **D** performs a **scaling** along the remapped orthogonal vectors depicted by a circle being stretched
  3. **P** undoes the basis change depicted as a **reverse rotation** and restores the original coordinate frame.



Example 4.11

$\boldsymbol{A} = \begin{bmatrix} 5/2 & -1 \\ -1 & 5/2 \end{bmatrix}$ Eigendecomposition of $\mathrm{A} = PDP^{-1}$?

$$\boldsymbol{A} = PDP^{-1} = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 7/2 & 0 \\ 0 & 3/2 \end{bmatrix} \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix}$$

Principal Component Analysis

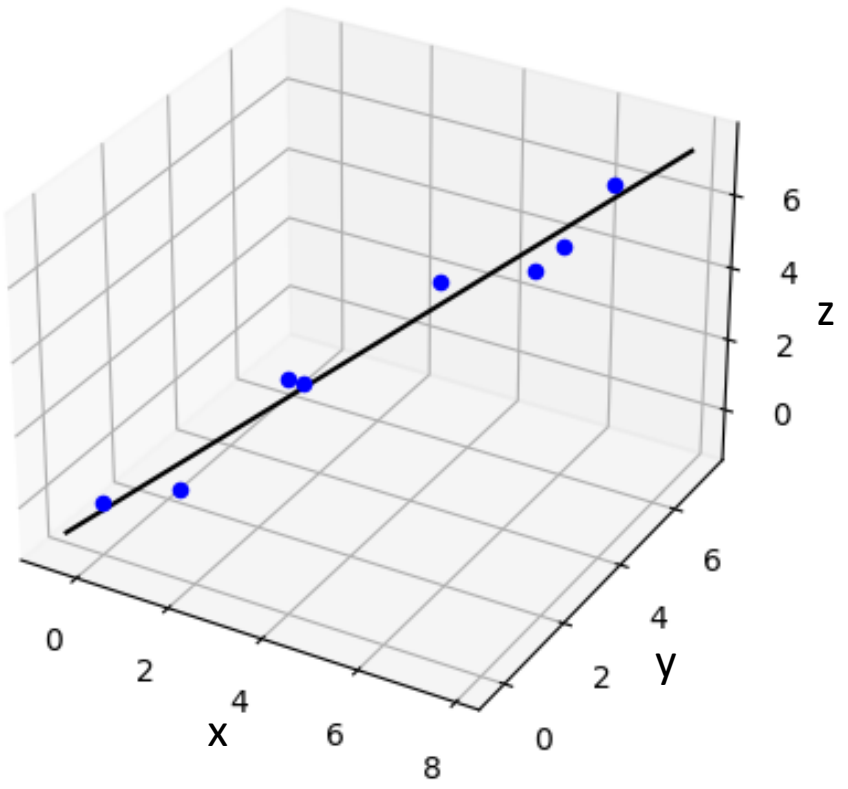
Readings:

- **Chapter 10 MML Textbook**

PCA

- Principle component analysis (PCA) is one example where eigendecomposition is used frequently
- Decomposing data in terms of factors has many benefits:
  - data interpretation
  - dimensionality reduction

Example



You can think of it as projections that maximize the variance in the data (i.e. information content).

These slides are adapted from

StatQuest

https://www.youtube.com/watch?v=FgakZw6K1QQ

Data

Samples!

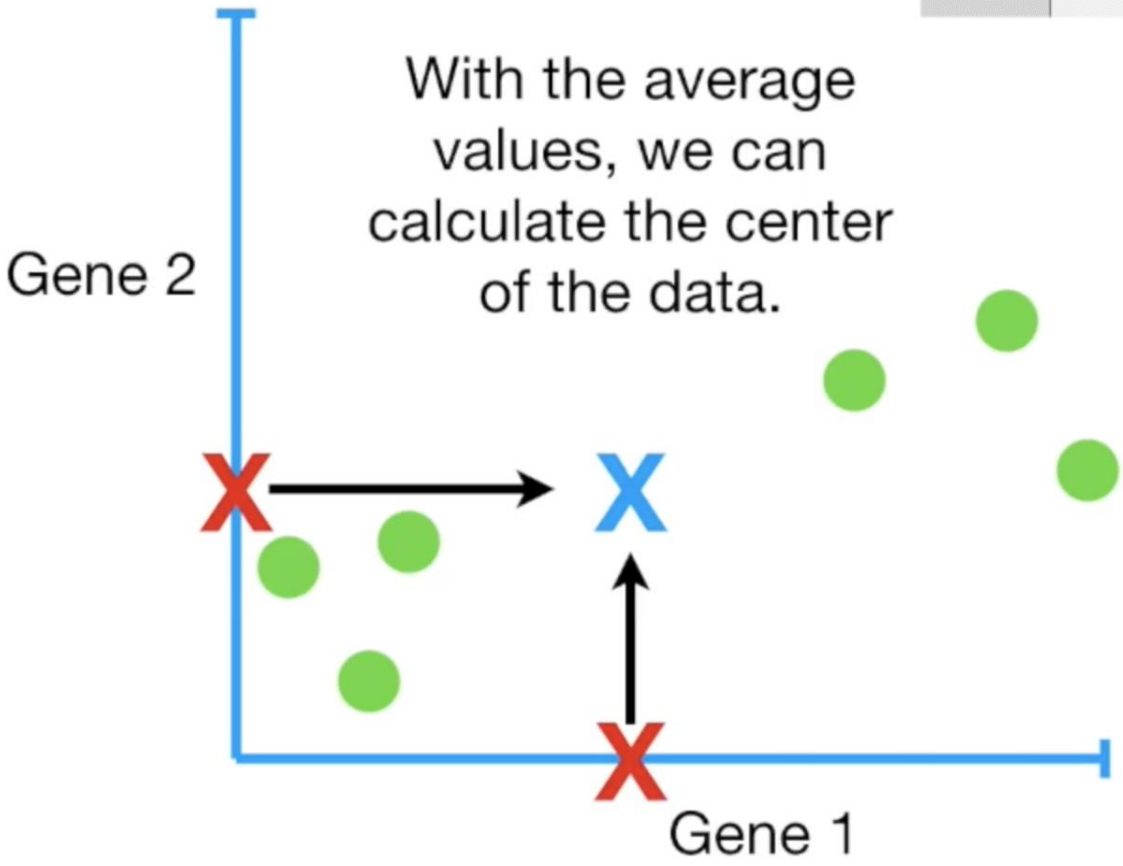
Variables!

	Mouse 1	Mouse 2	Mouse 3	Mouse 4	Mouse 5	Mouse 6
Gene 1	10	11	8	3	2	1
Gene 2	6	4	5	3	2.8	1

We can plot 2 variables in 2D.

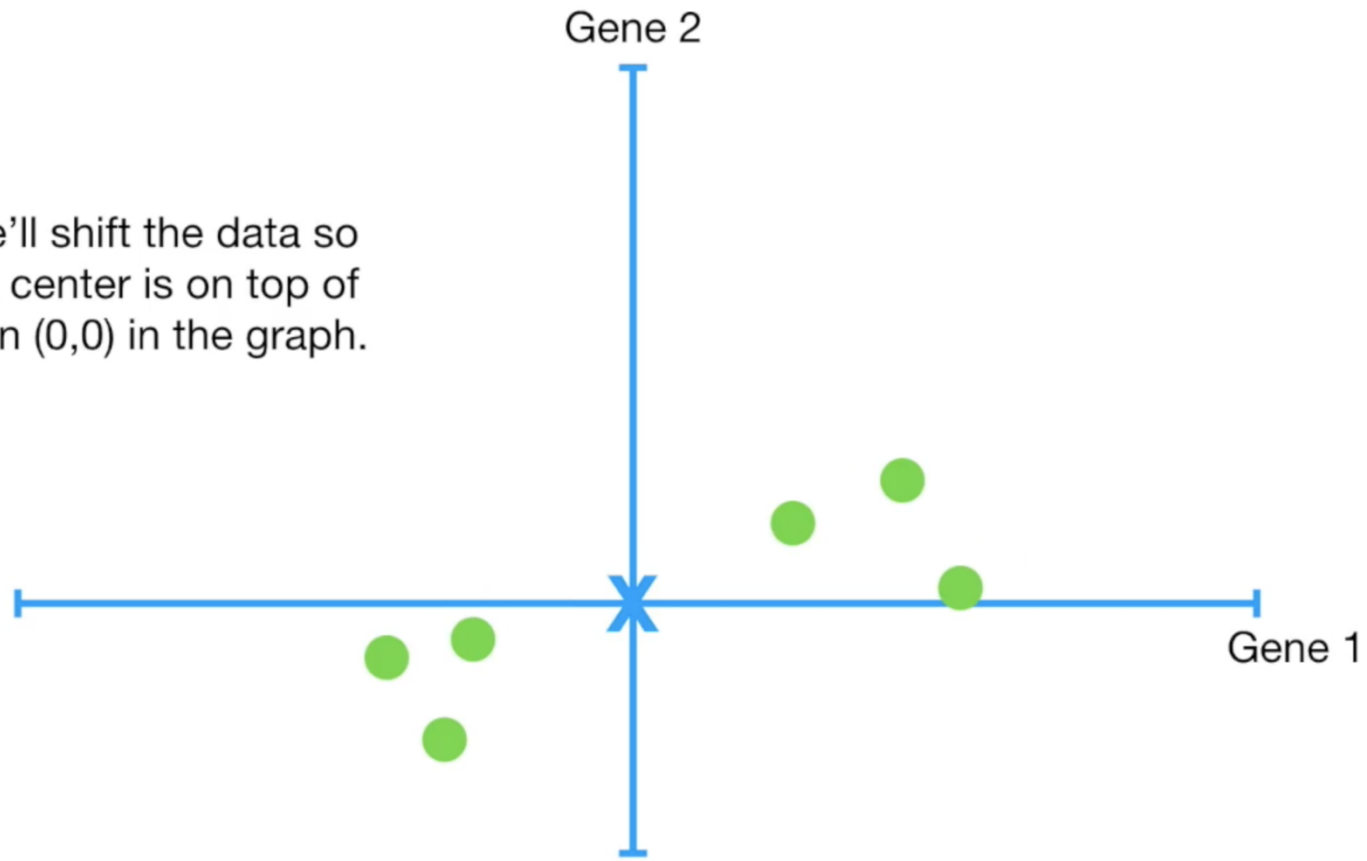
Average

	Mouse 1	Mouse 2	Mouse 3	Mouse 4	Mouse 5	Mouse 6
Gene 1	10	11	8	3	2	1
Gene 2	6	4	5	3	2.8	1

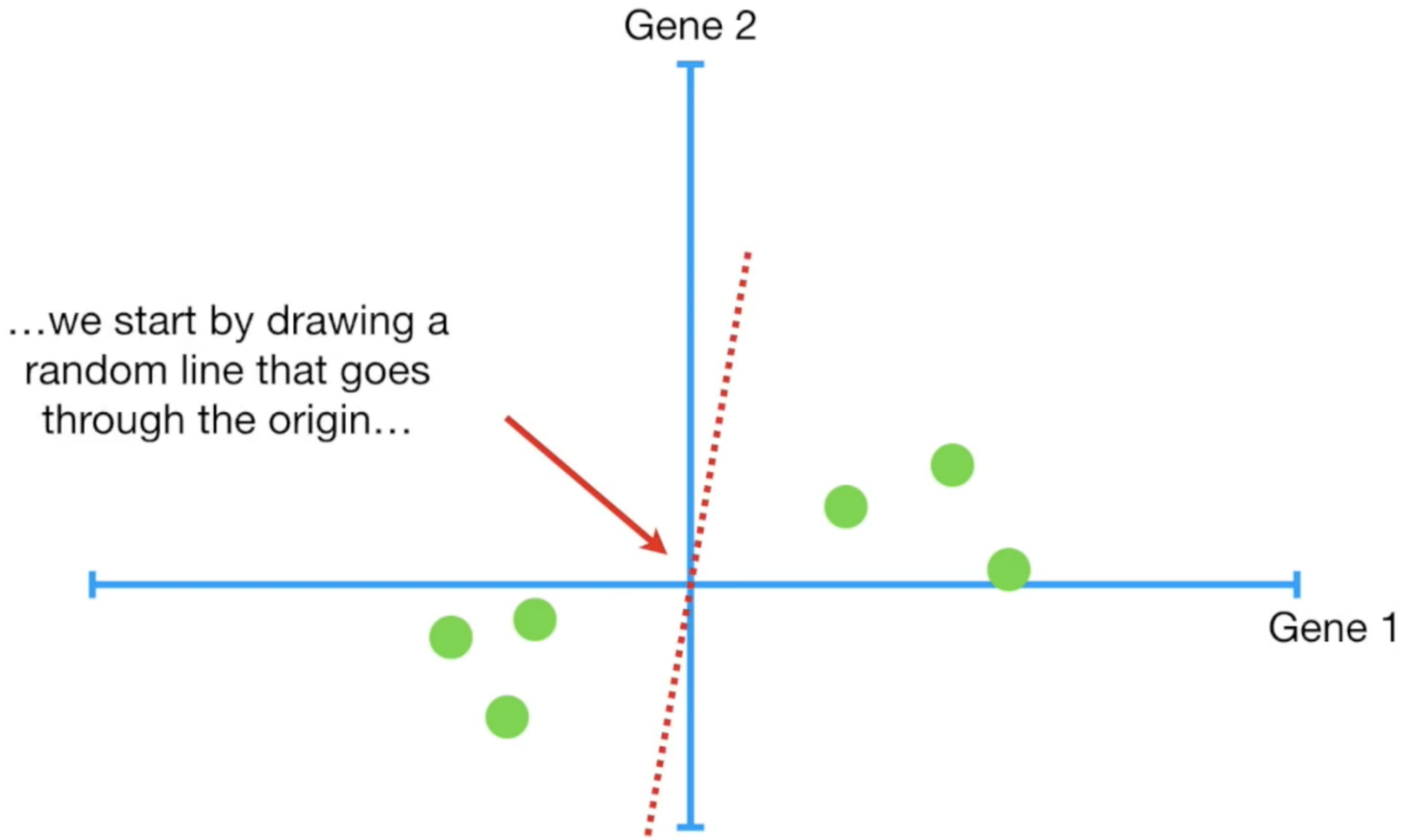


Shift the data

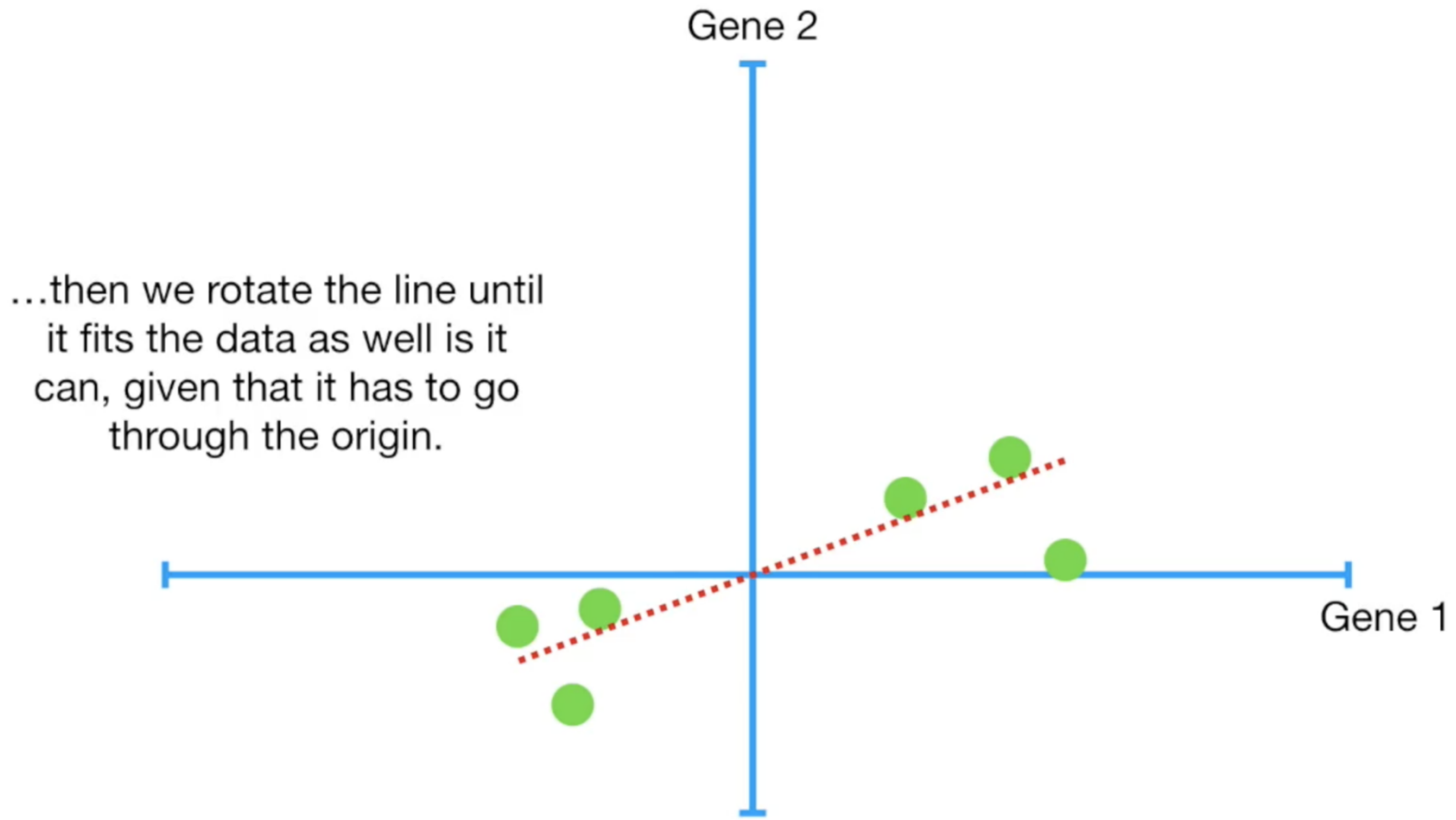
Now we'll shift the data so that the center is on top of the origin (0,0) in the graph.



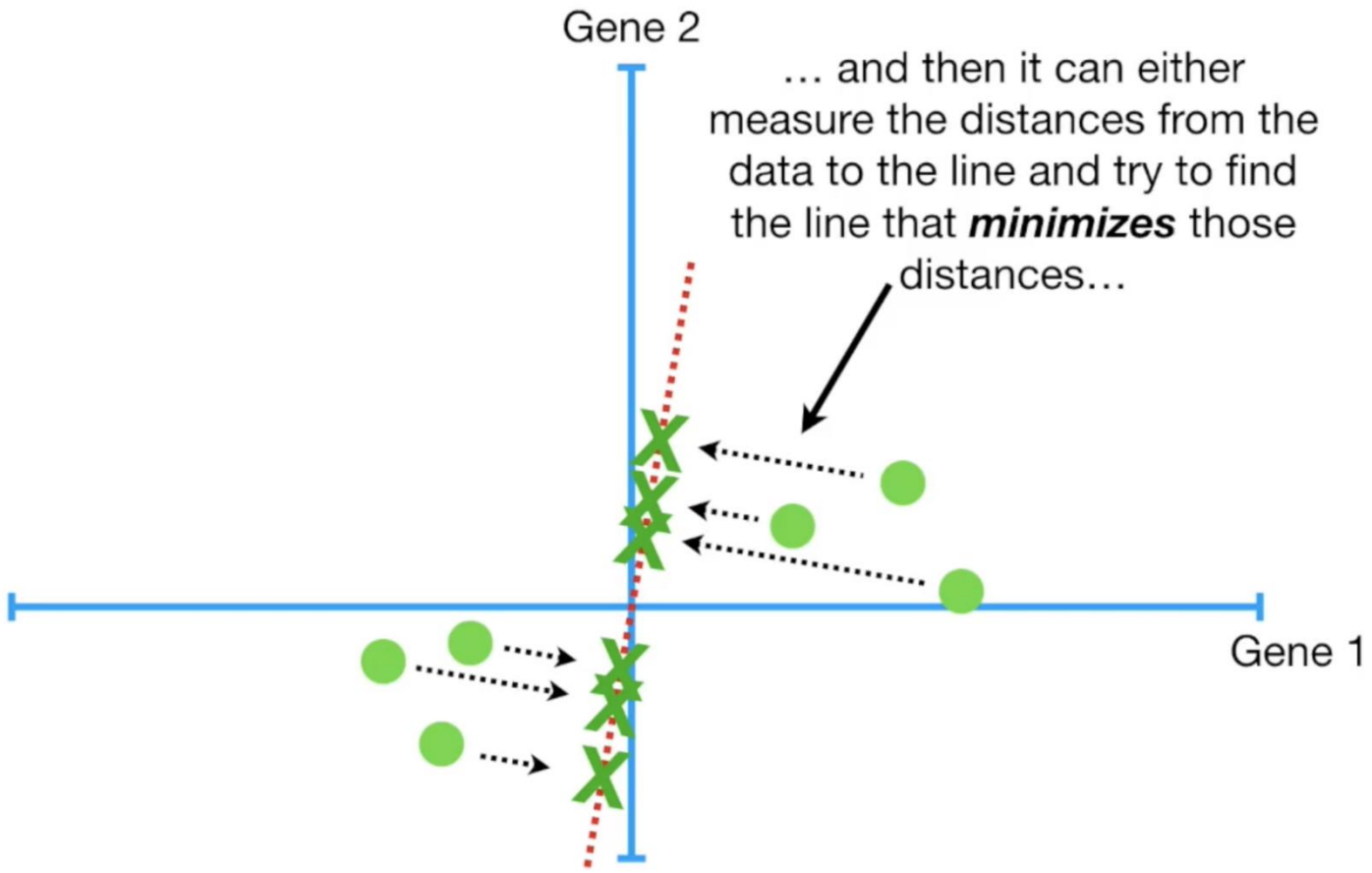
Draw a line crossing the origin



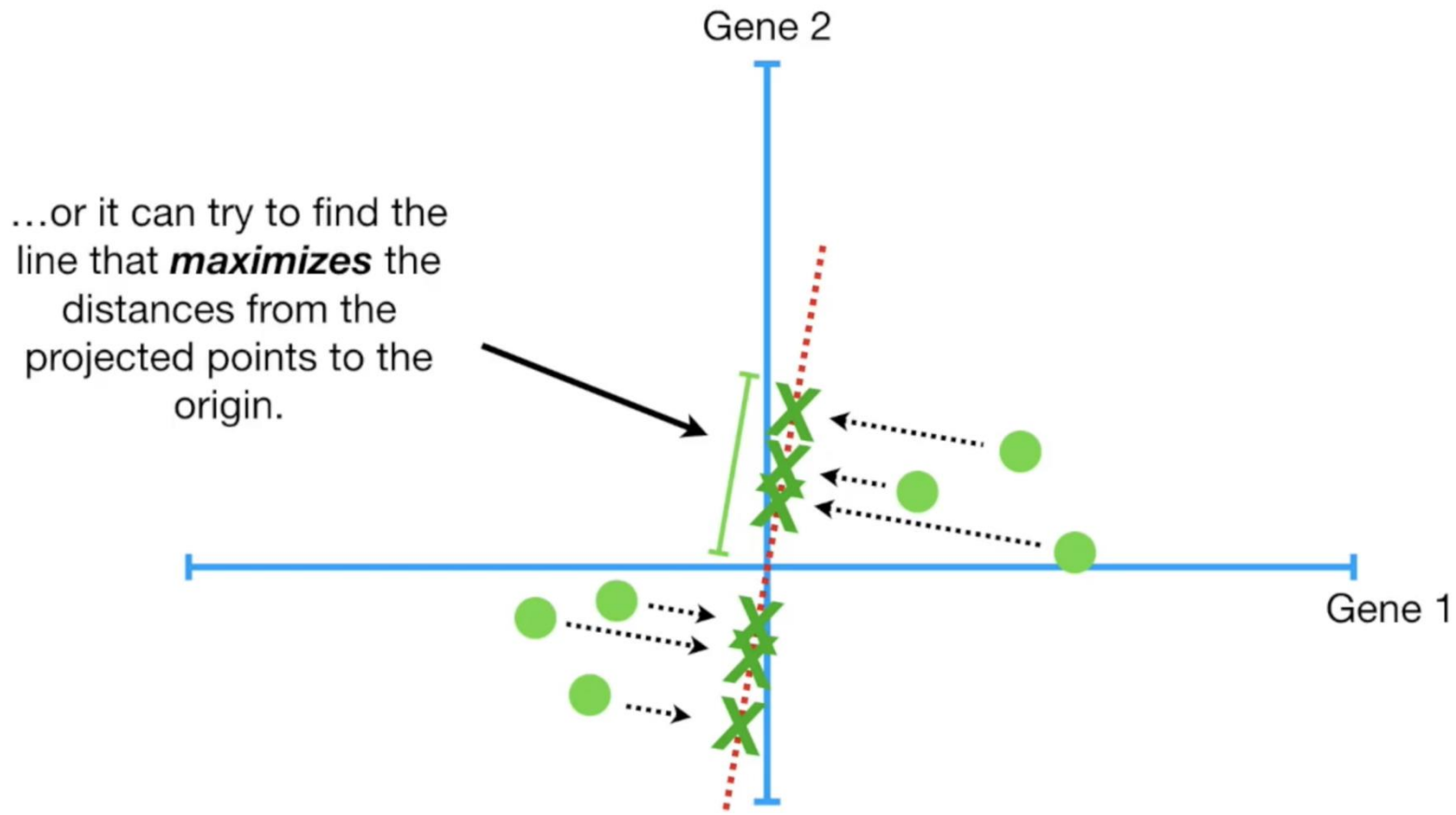
Goal: Fit the data as best as a line can



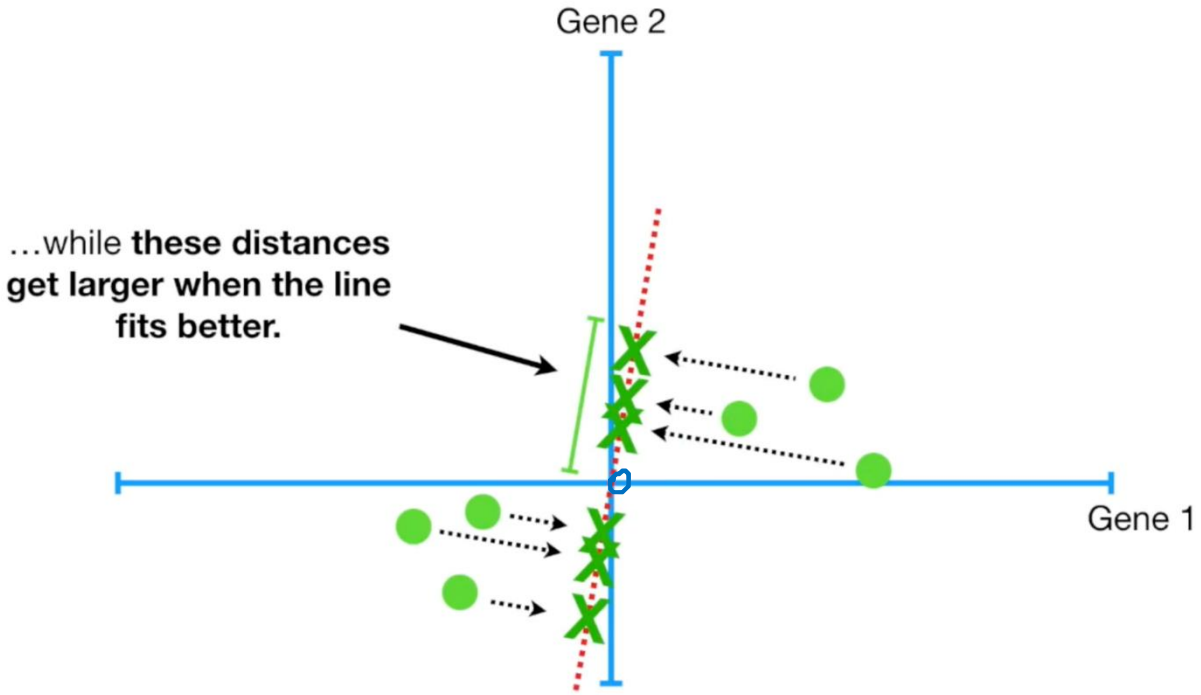
How do we know we have the best fit?

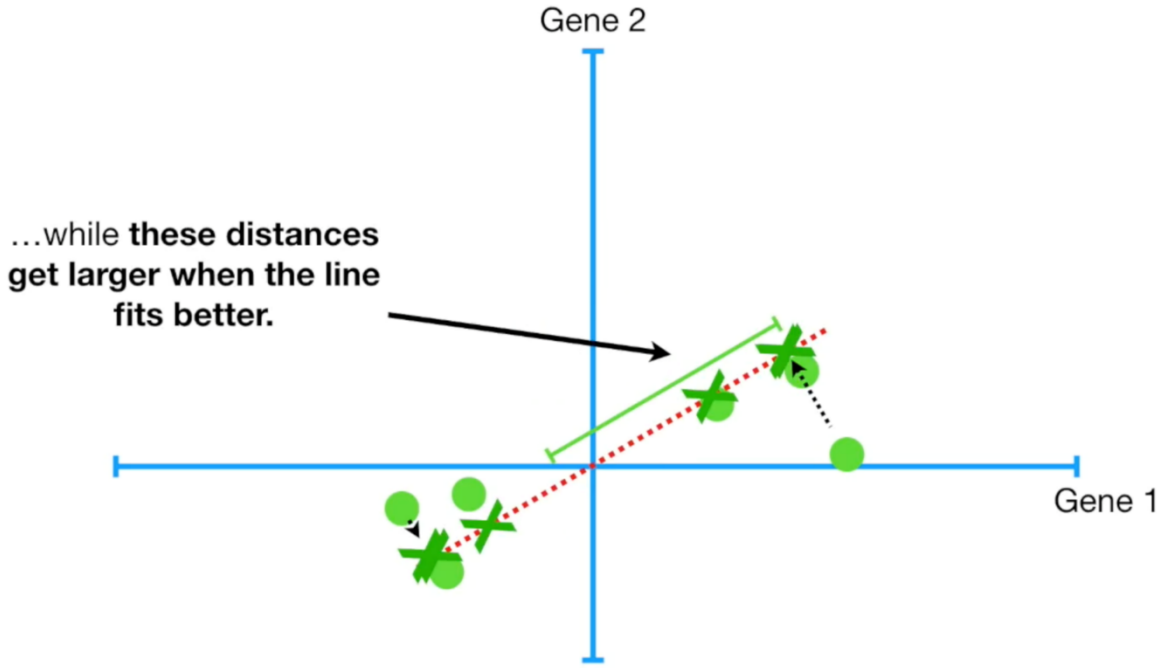


How we know the best fit?



Intuition

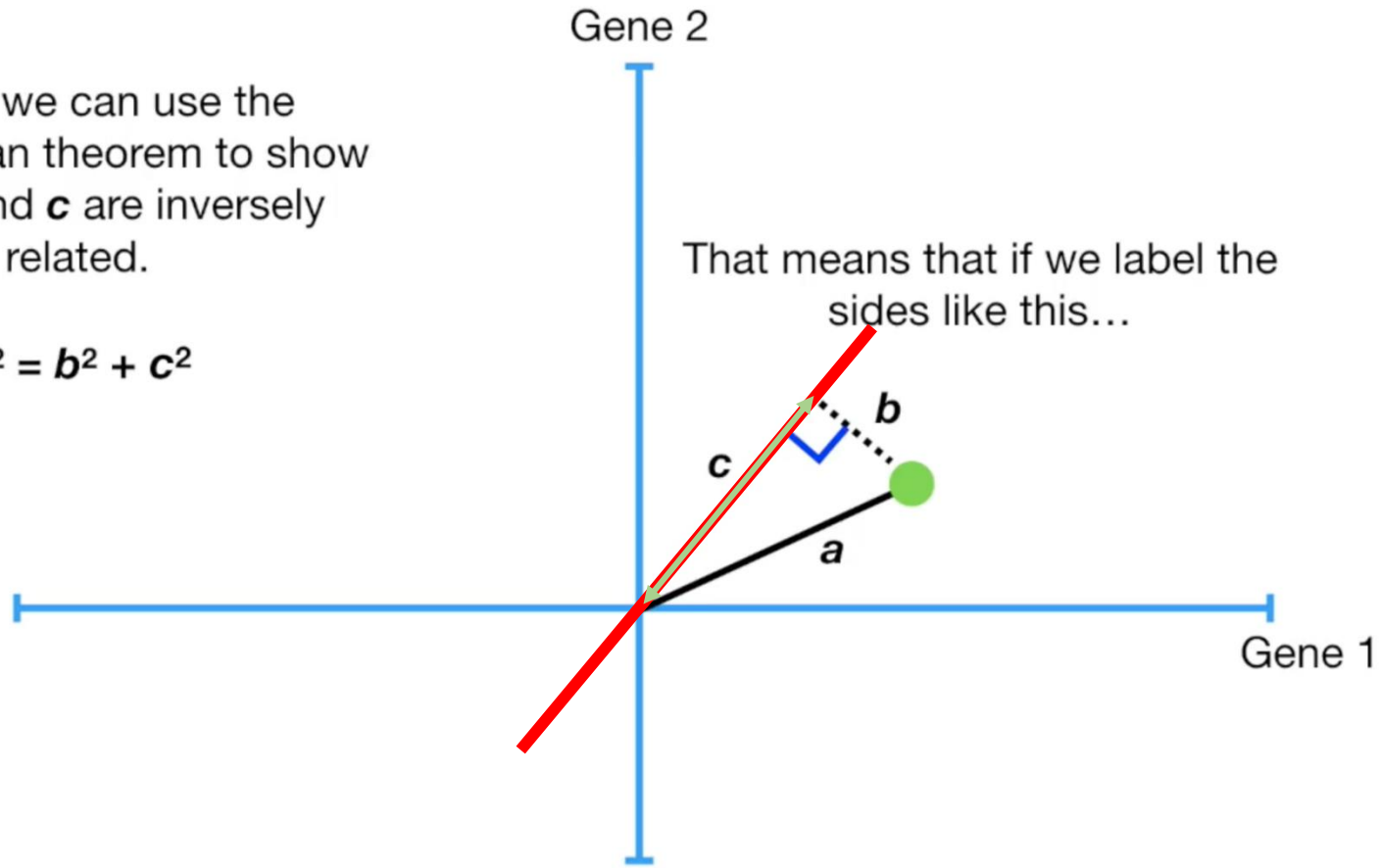

Gene 2
…while these distances get larger when the line fits better.
Gene 1


Gene 2
…while these distances get larger when the line fits better.
Gene 1

Why?

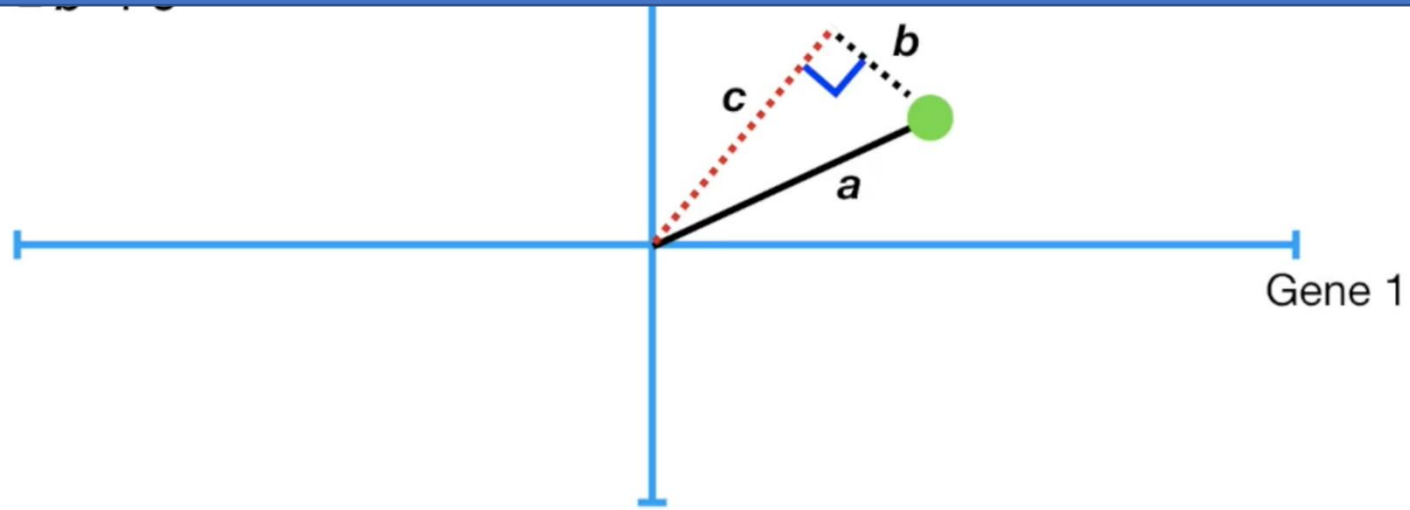
…then we can use the Pythagorean theorem to show how ***b*** and ***c*** are inversely related.

$$a^2 = b^2 + c^2$$

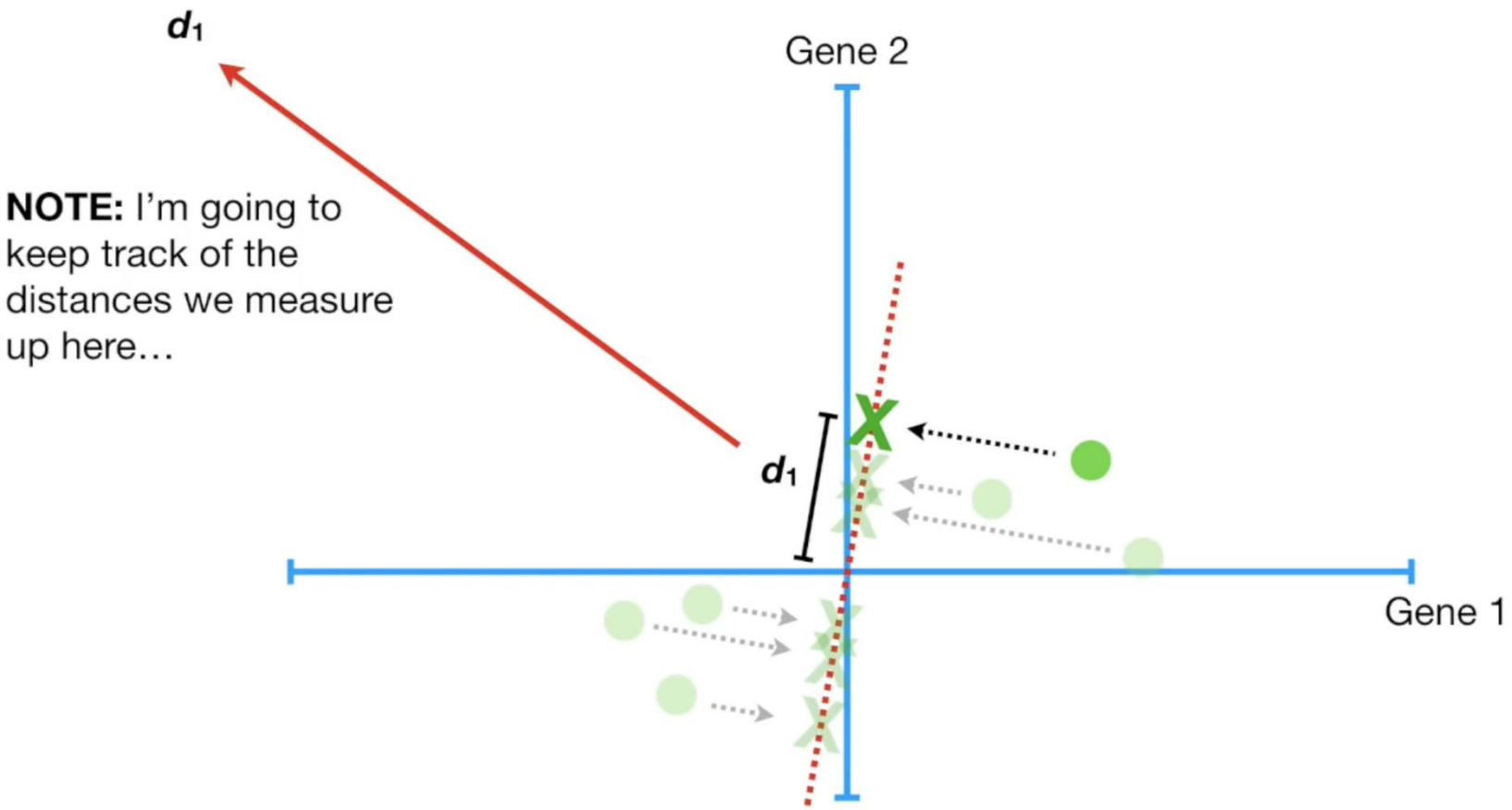


Why?

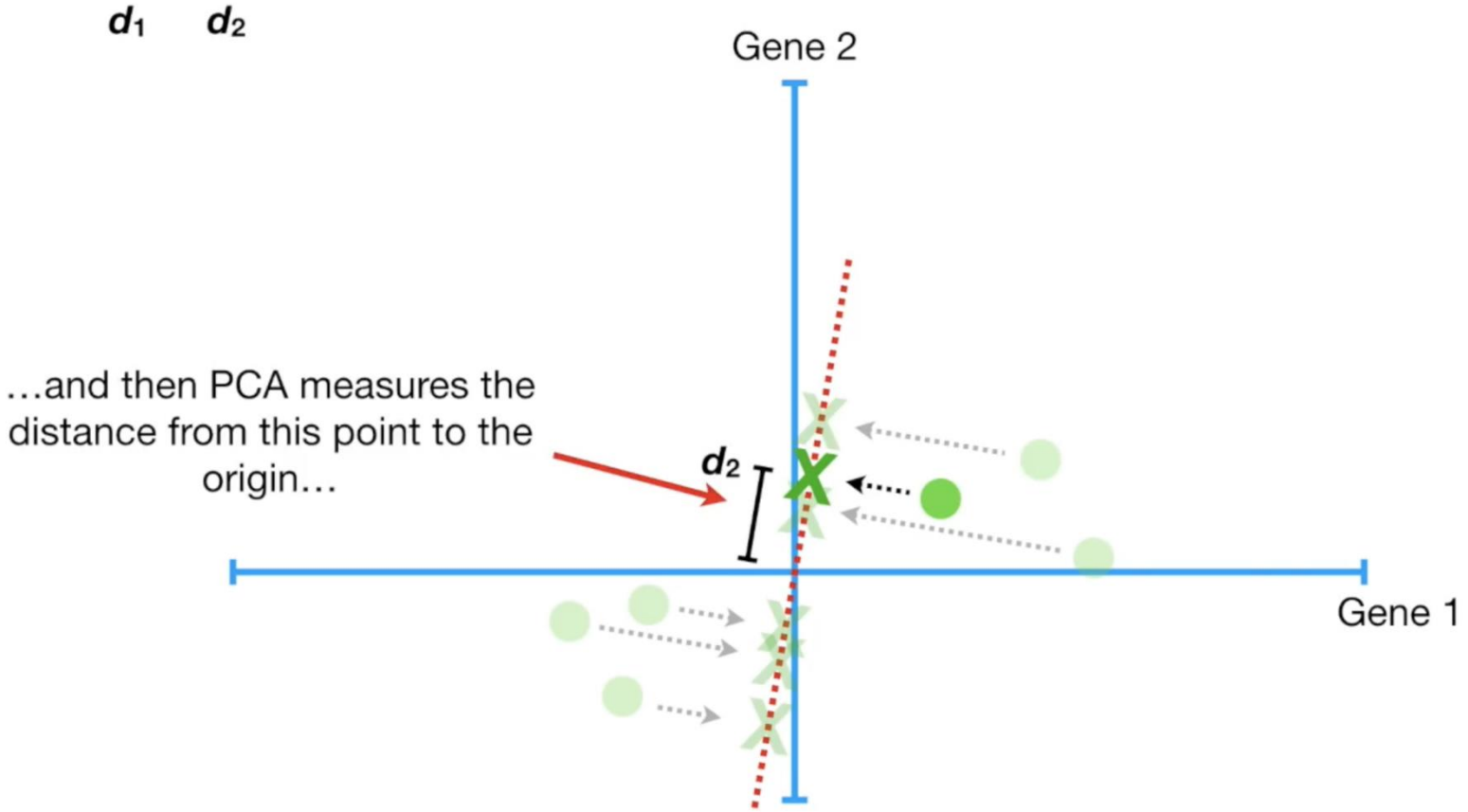
Objective: Minimize b or Maximize c



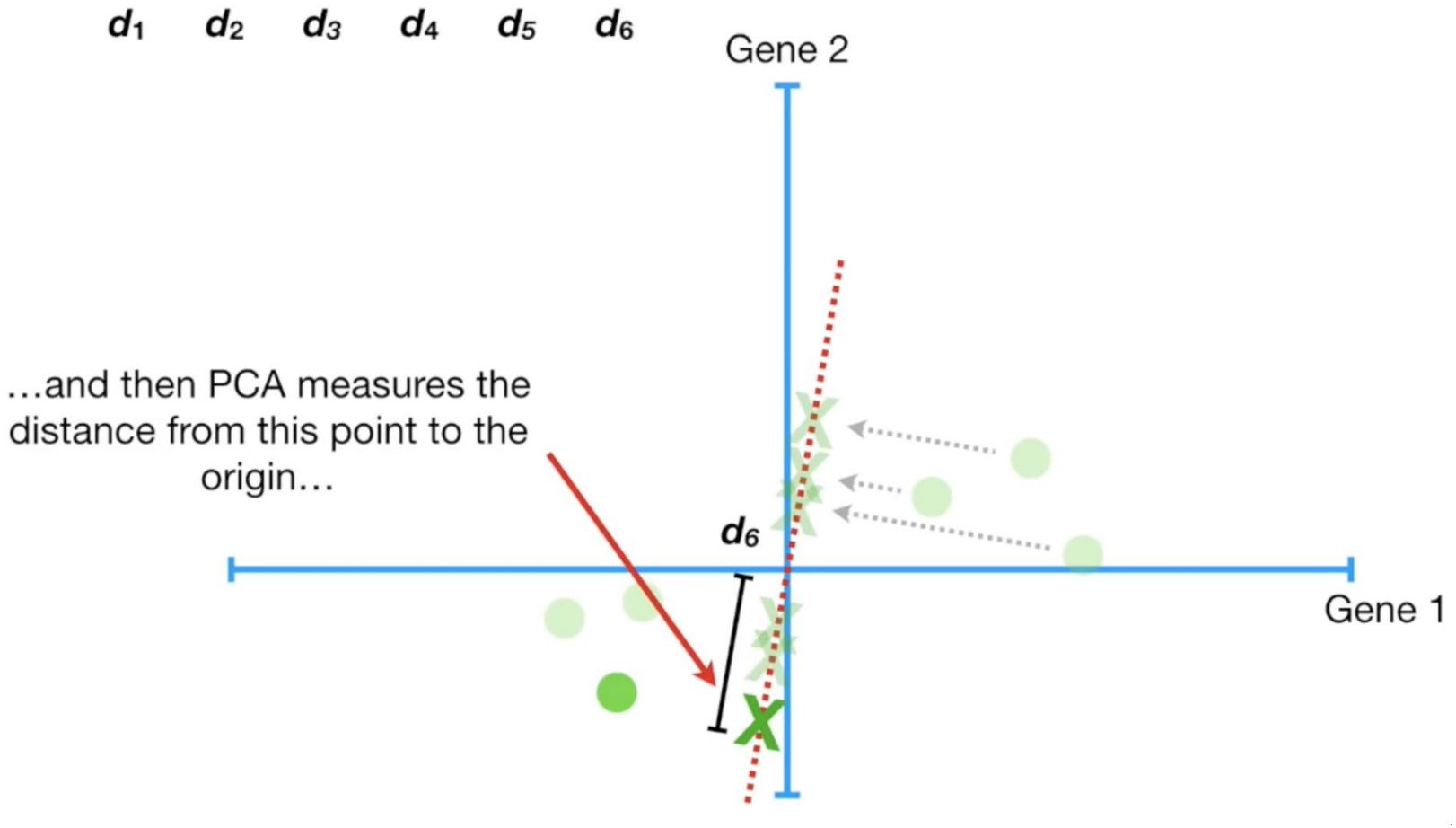
Distances


d_1
NOTE: I'm going to keep track of the distances we measure up here…
Gene 2
d_1
Gene 1

Distances

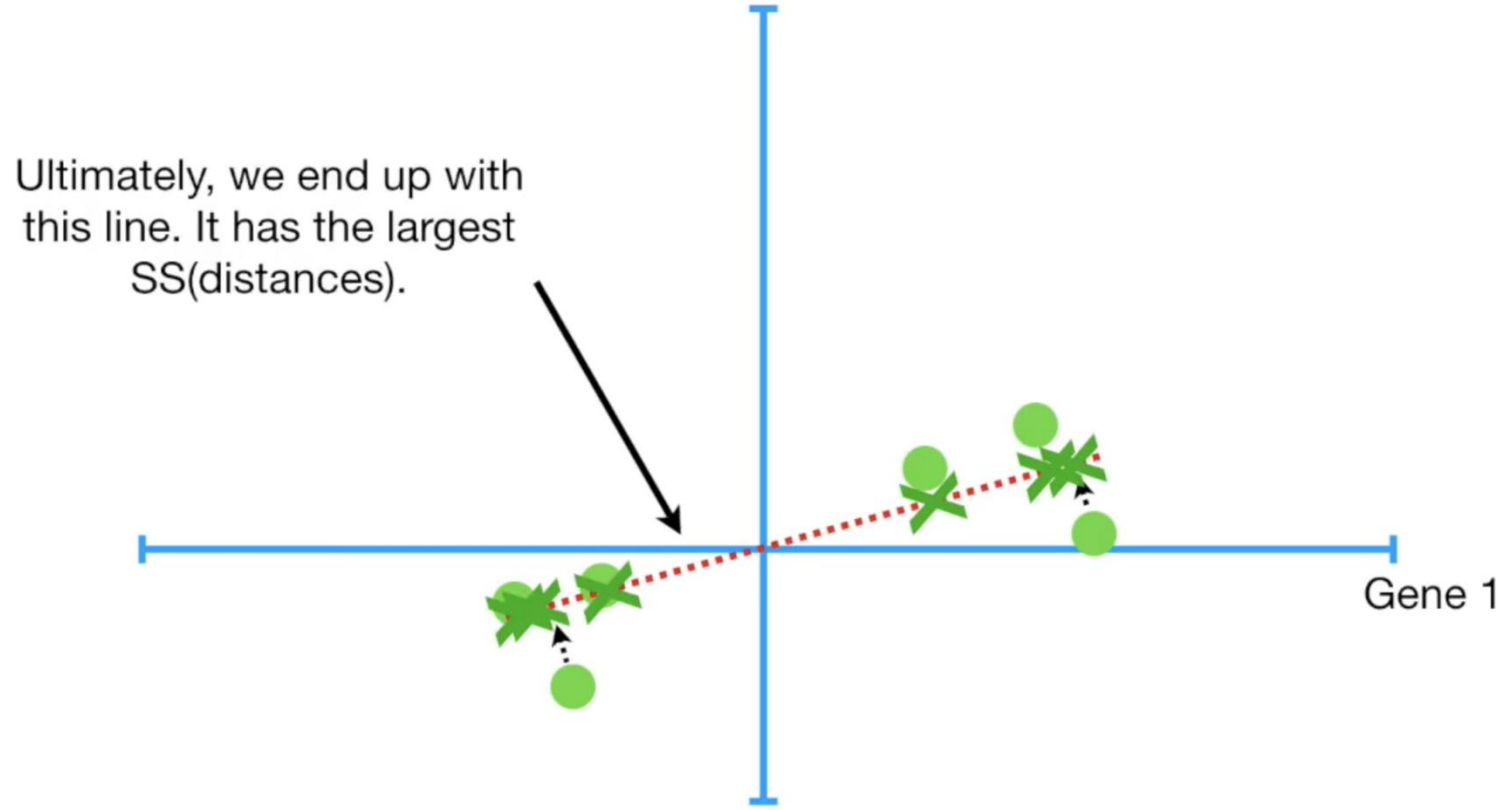

d_1
d_2
Gene 2
…and then PCA measures the distance from this point to the origin…
d_2
Gene 1

Distances

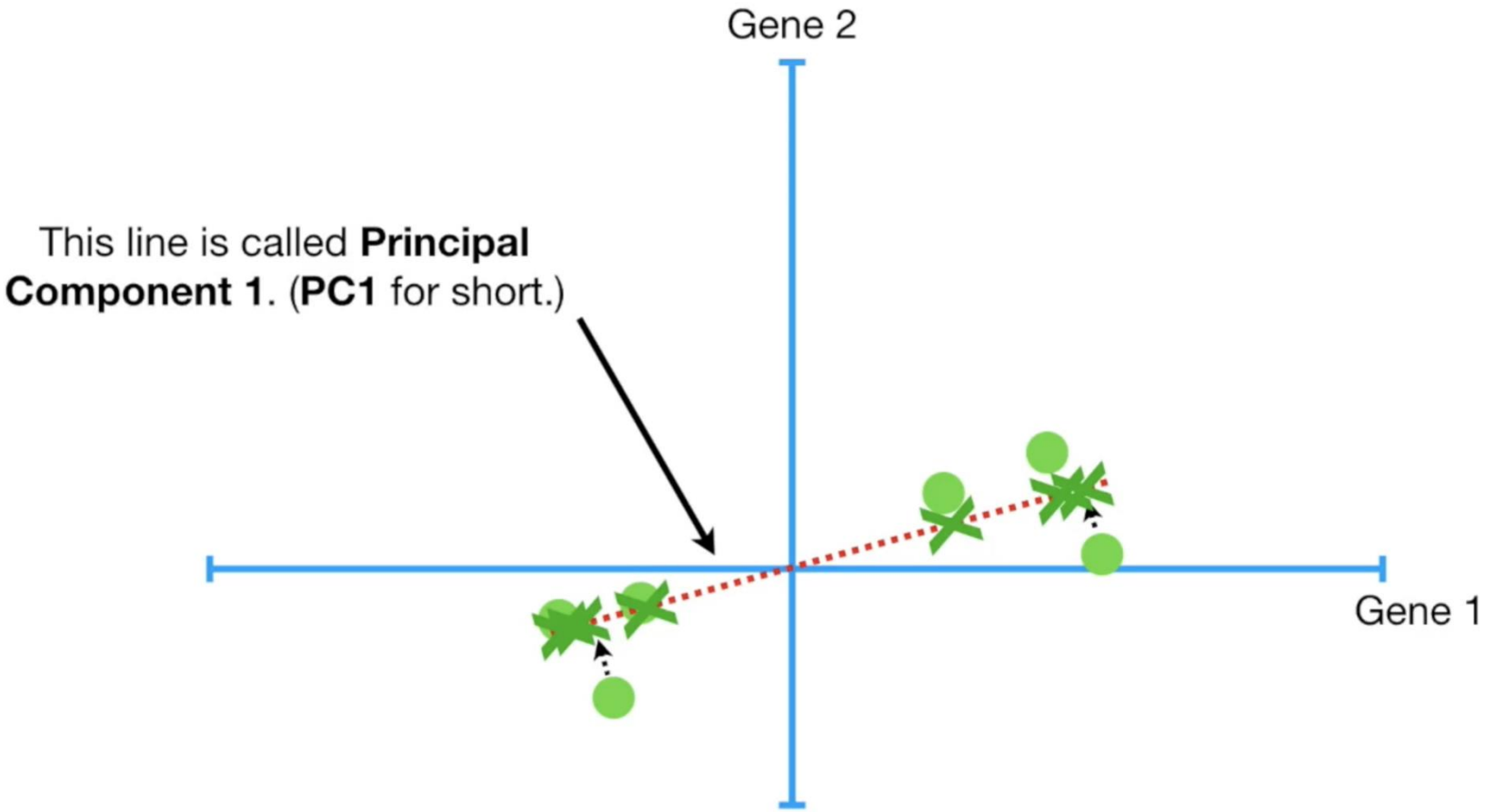

d_1 d_2 d_3 d_4 d_5 d_6
Gene 2
…and then PCA measures the distance from this point to the origin…
d_6
Gene 1

Maximize the Sum of squared distances

$d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2$ = sum of squared distances = SS(distances)



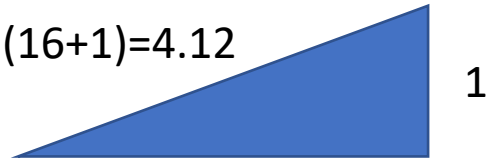
First Principal Component



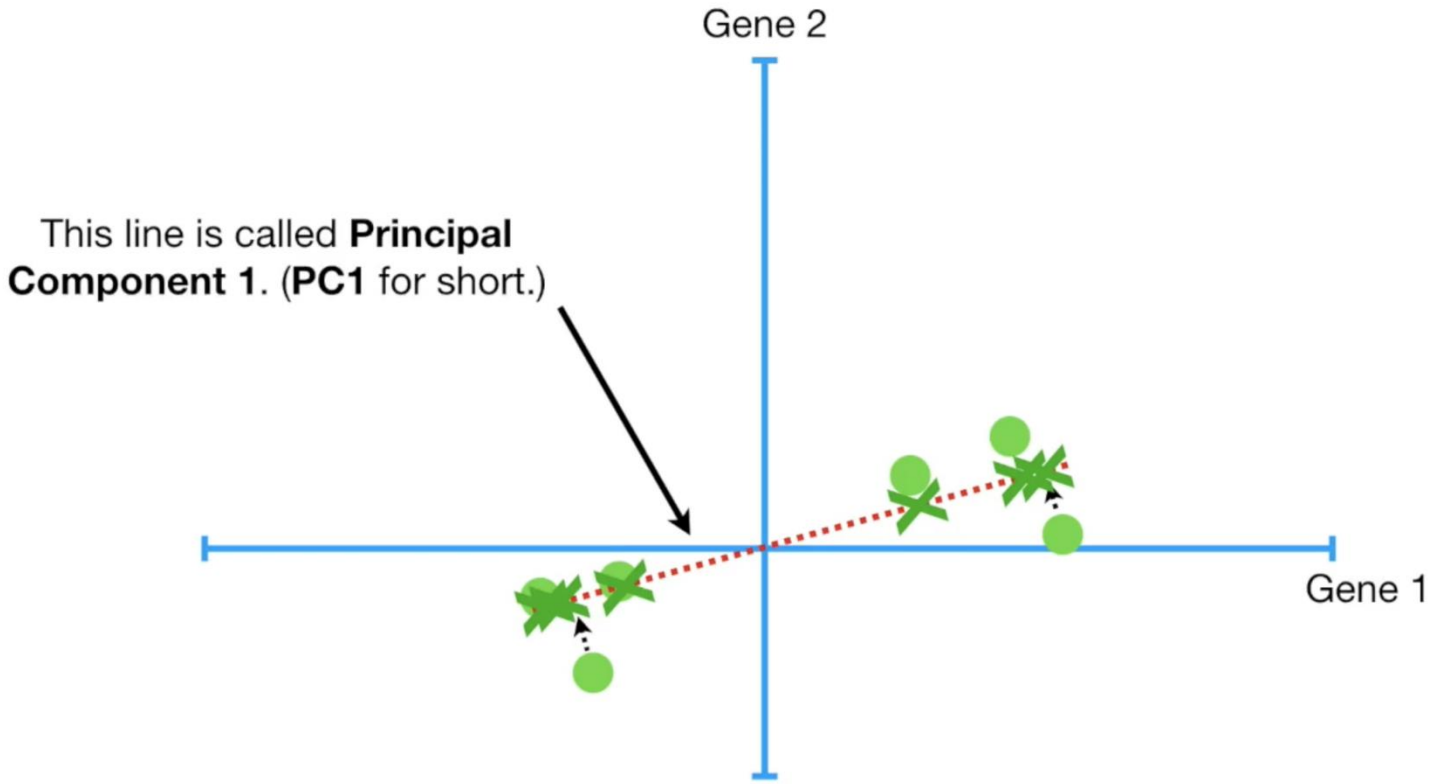
First Principal Component

The slope of the PC1 = 0.25

Sqrt (16+1)=4.12

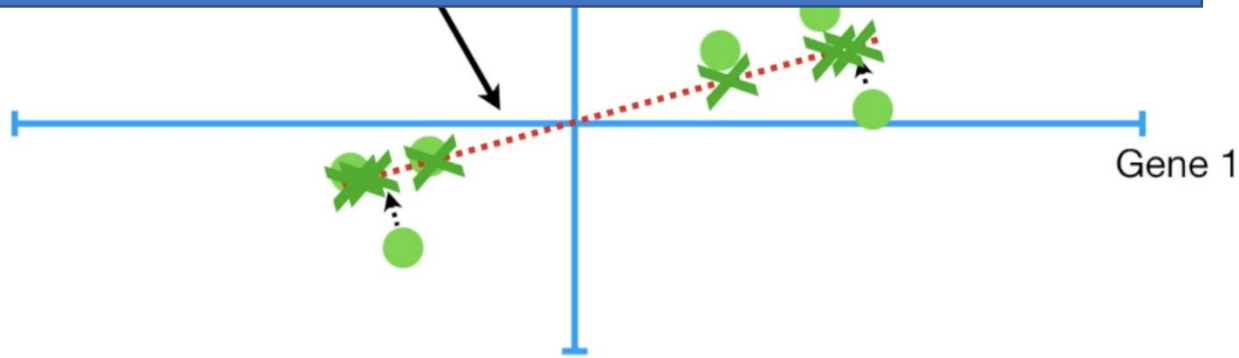


Norm



First Principal Component

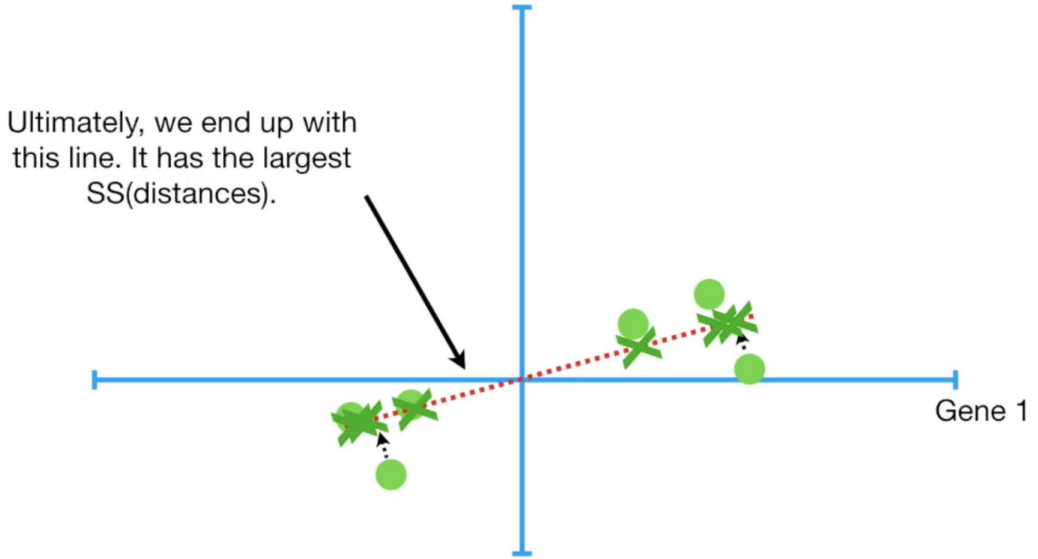
Eigenvector for PC1 = [0.97, 0.242]
Other name: Singular vector



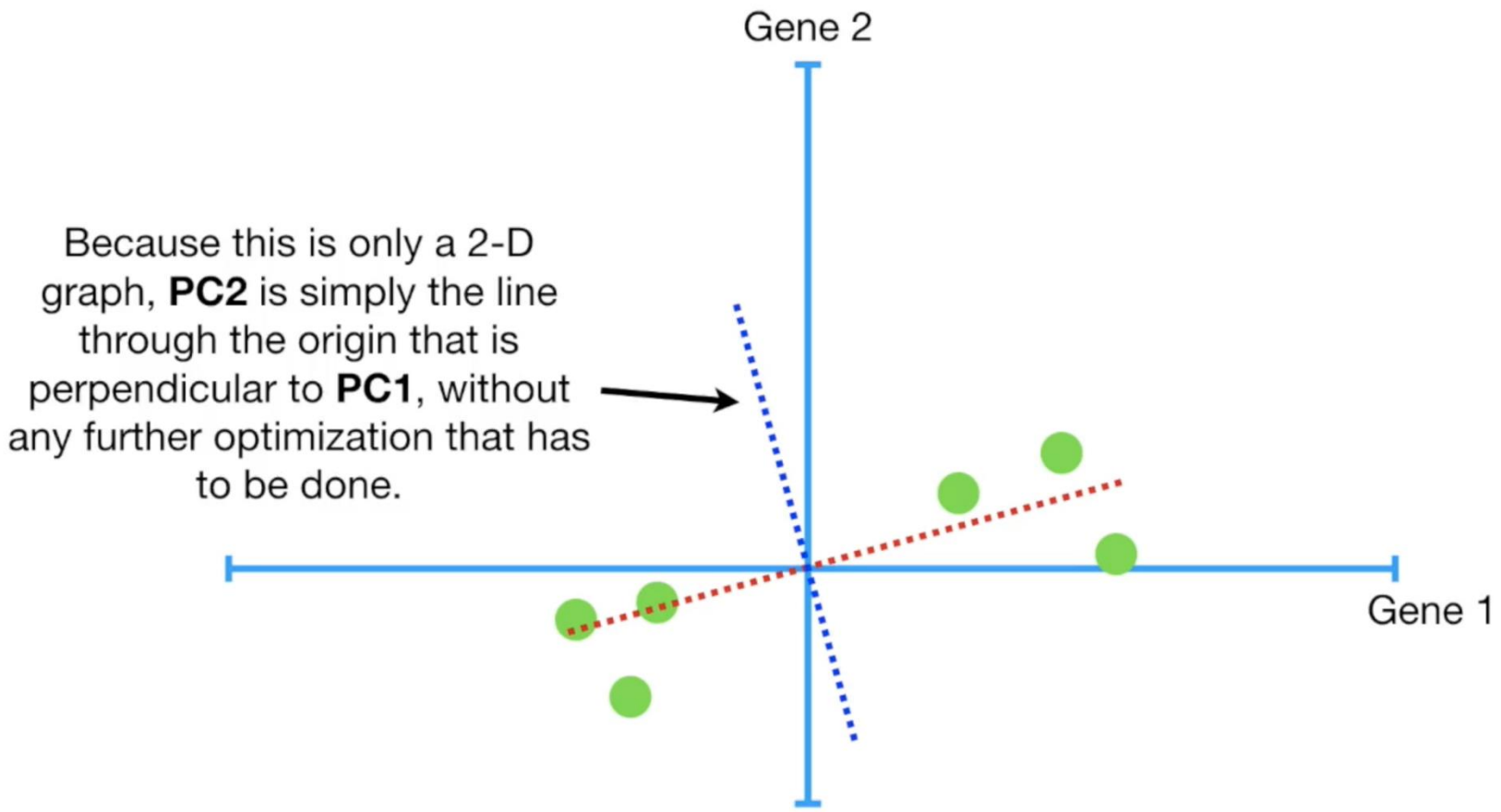
First Principal Component

Sum of squared distances for PC1 = **Eigenvalue** for PC1
Sqrt(Eigenvalue for PC1) = Singular Value for PC1

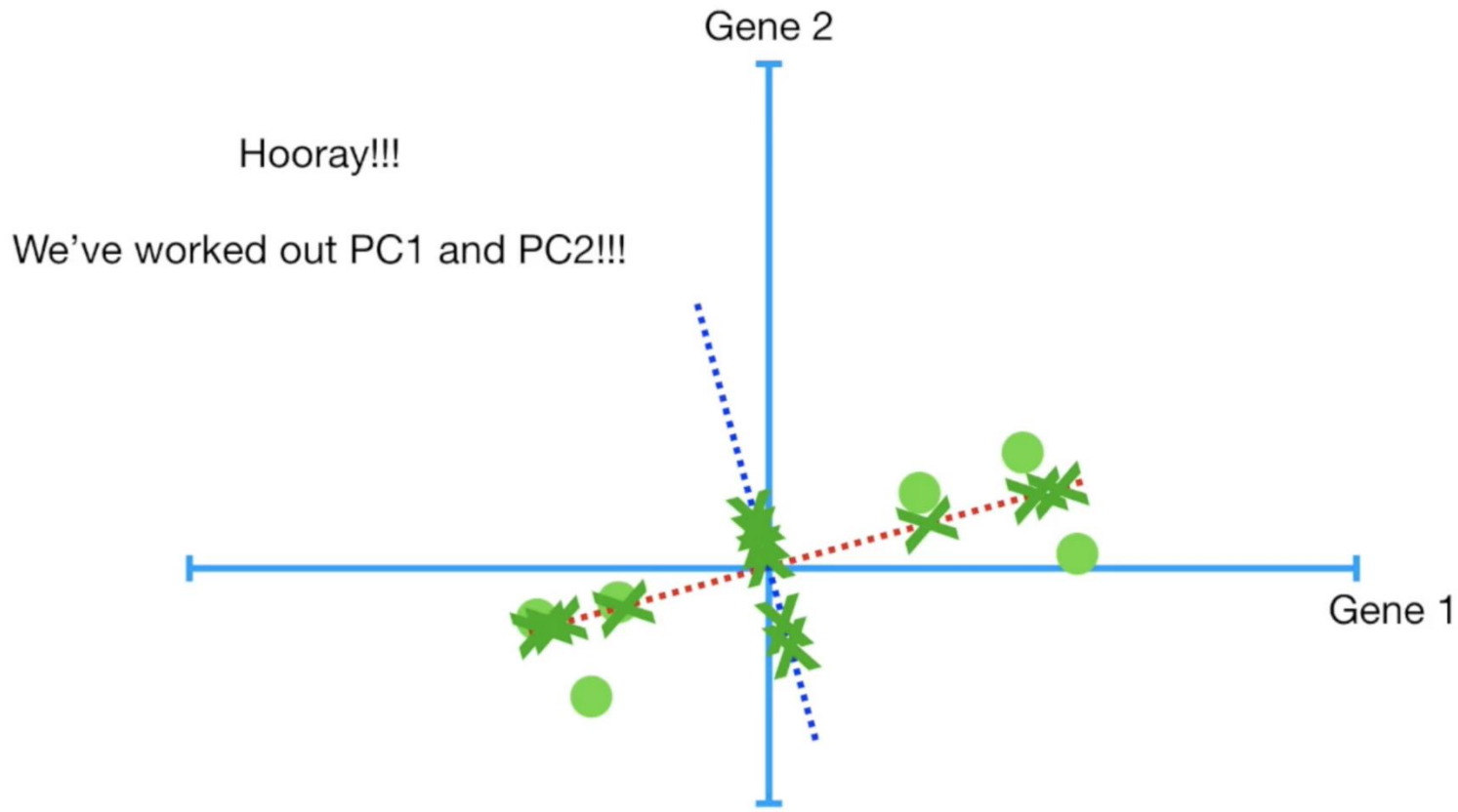
$d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2$ = sum of squared distances = SS(distances)



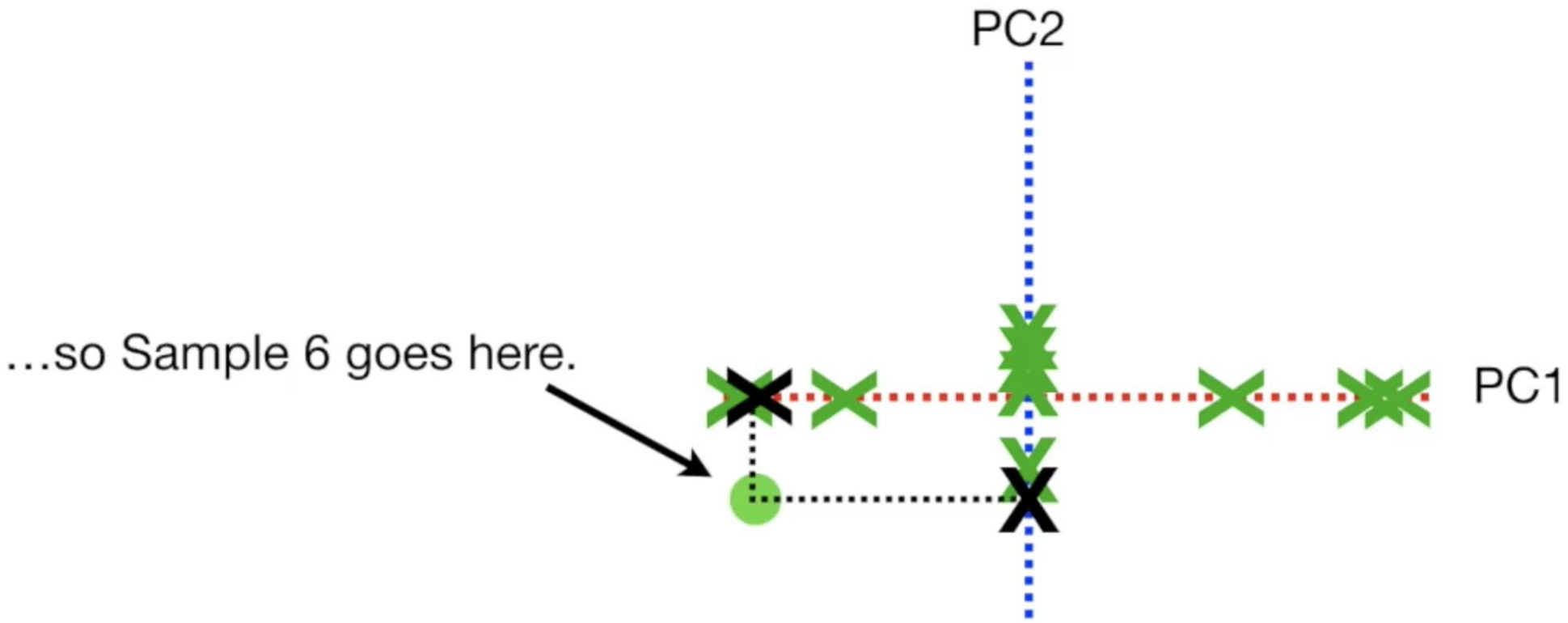
PC2


Gene 2
Because this is only a 2-D graph, **PC2** is simply the line through the origin that is perpendicular to **PC1**, without any further optimization that has to be done.
Gene 1

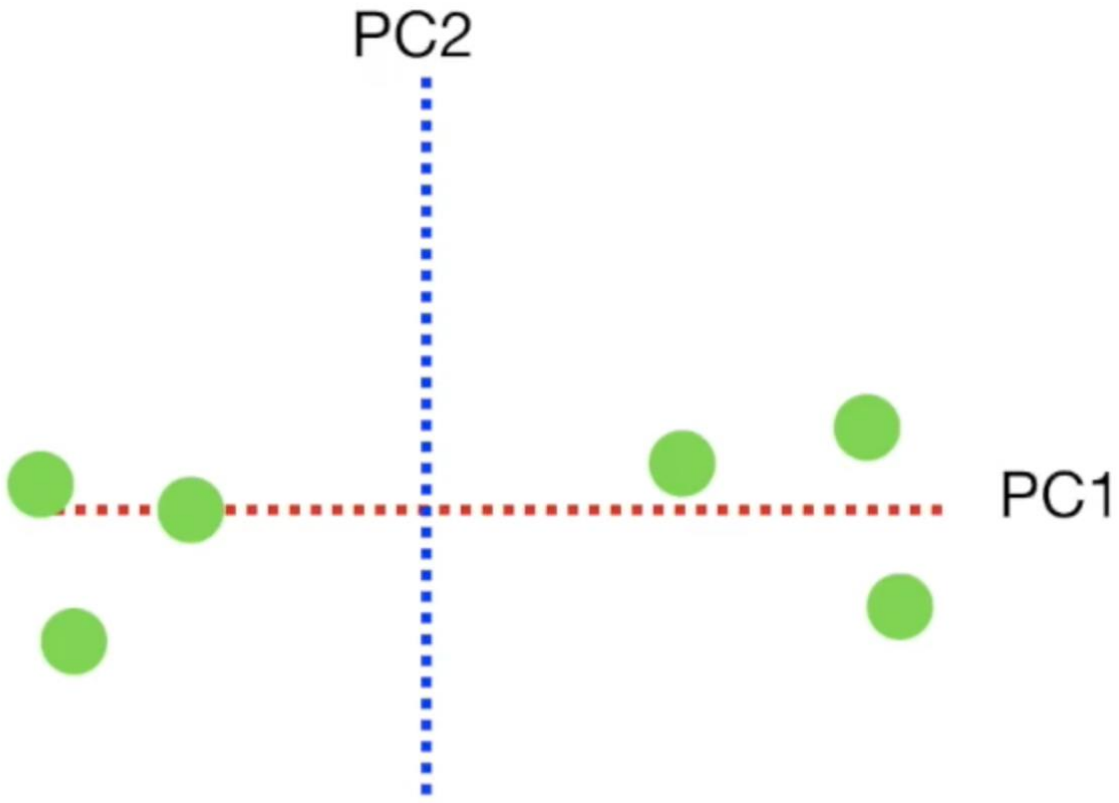
Projection - PC1 and PC2



Reconstruction

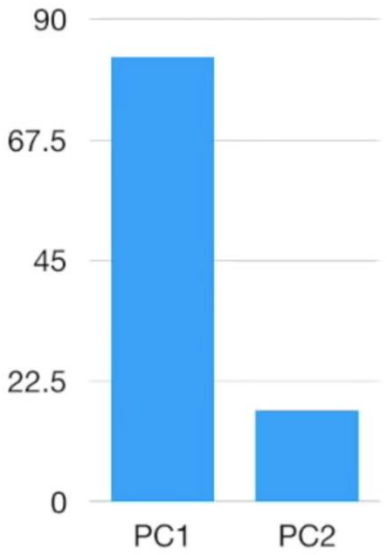


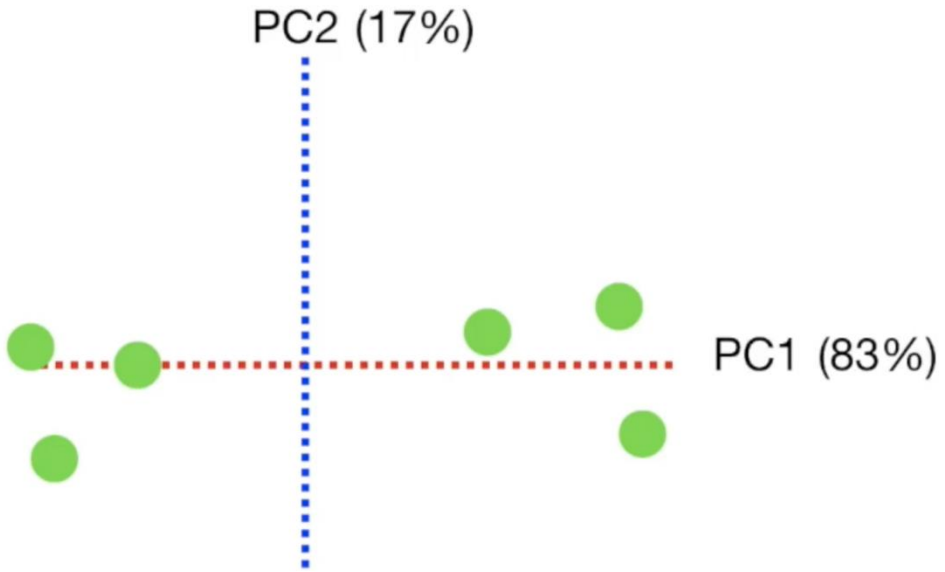
Reconstruction



Scree Plot

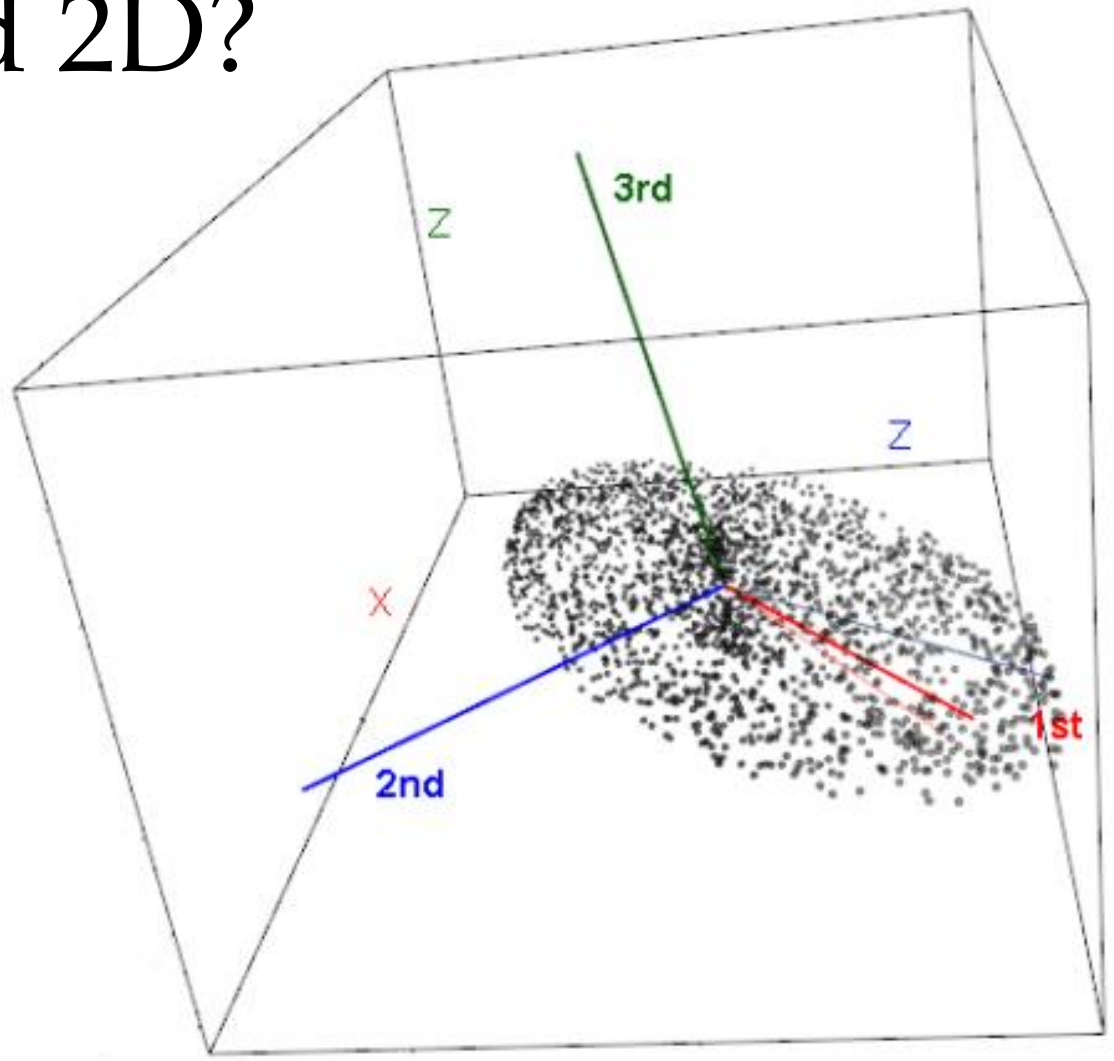
TERMINOLOGY ALERT!!!! A **Scree Plot** is a graphical representation of the percentages of variation that each PC accounts for.





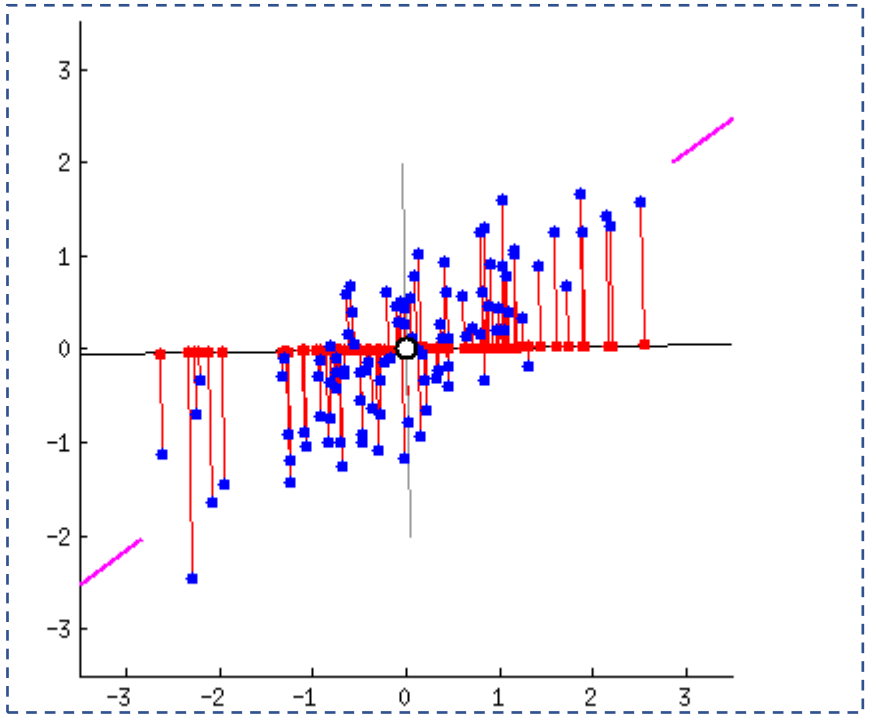
What happens beyond 2D?

- Rigidly rotate the coordinate axes to new (principal axes) such that:
  - principal axis 1 corresponds to the highest variance,
  - axis 2 has the next highest variance,
  - . . . ,
  - and axis *p* has the lowest variance.
  - All principal axes are uncorrelated (orthogonal).

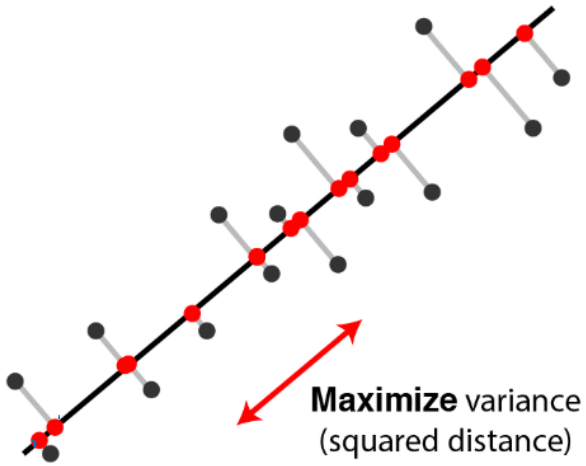


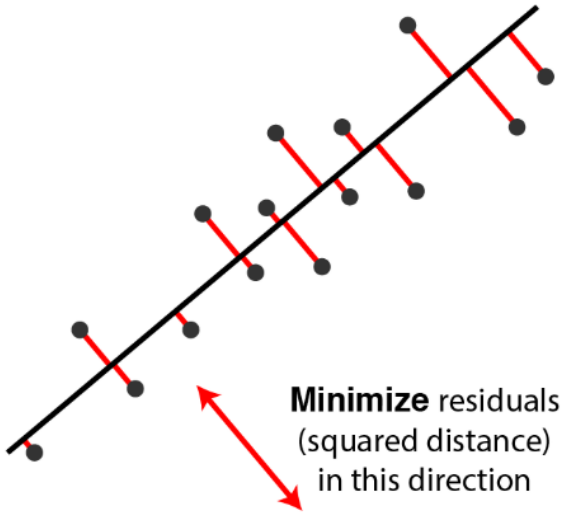
Source: Václav Hlaváč

In Summary…



Source: Stackoverflow





Source: Alex Williams

- Project D-dimensional data onto an M-dimensional subspace that retains as much information as possible
- Informally: information = diversity = variance

PCA Algorithm Overview

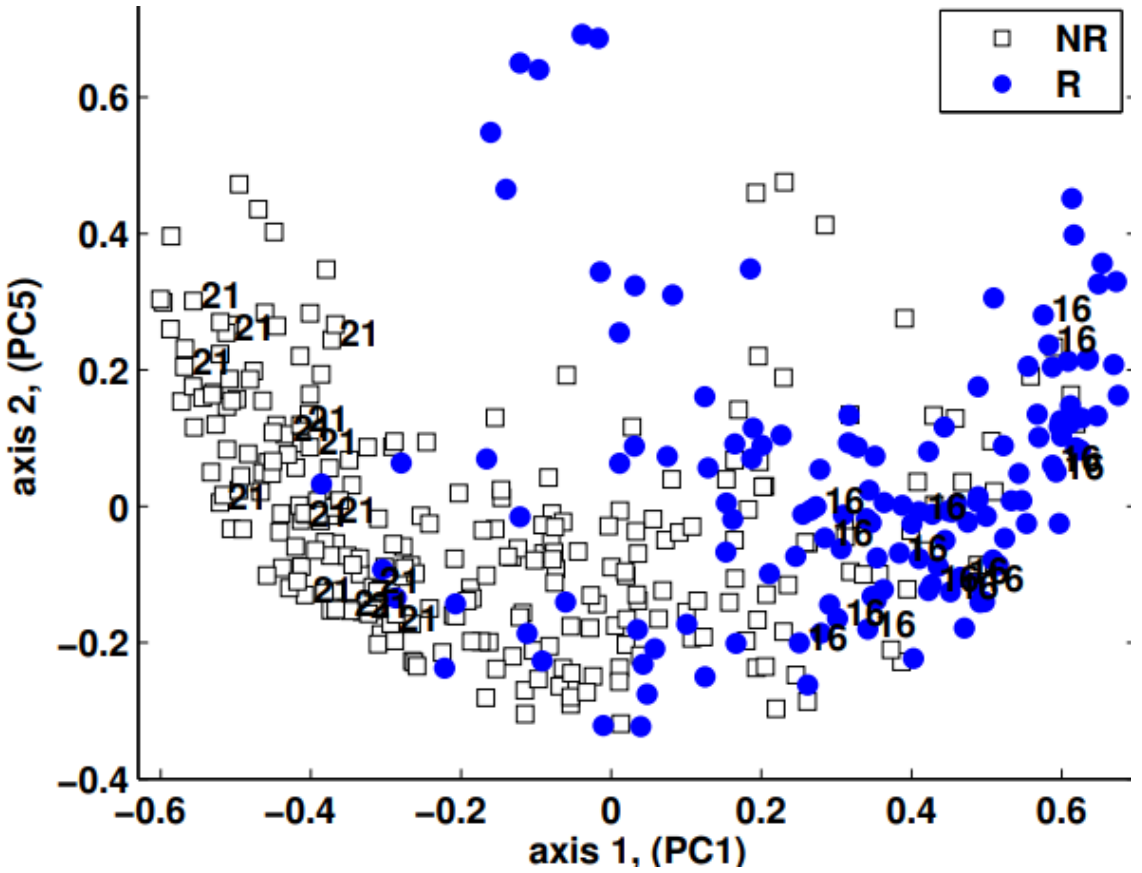
1. Standardize the data (zero mean) and compute the covariance matrix
2. Obtain the Eigenvectors and Eigenvalues of the covariance matrix
3. Choose the k eigenvectors that correspond to the k largest eigenvalues
4. Construct the projection matrix $\mathbf{W}$ from the selected k eigenvectors.
5. Transform the original dataset $\mathbf{X}$ via $\mathbf{W}$ to obtain a k-dimensional feature subspace $\mathbf{Y}$. (=**X@W**)

→ **interpretation of data** by examining principal components

→ discard components for **dimensionality reduction**

Visualization of Principle Components

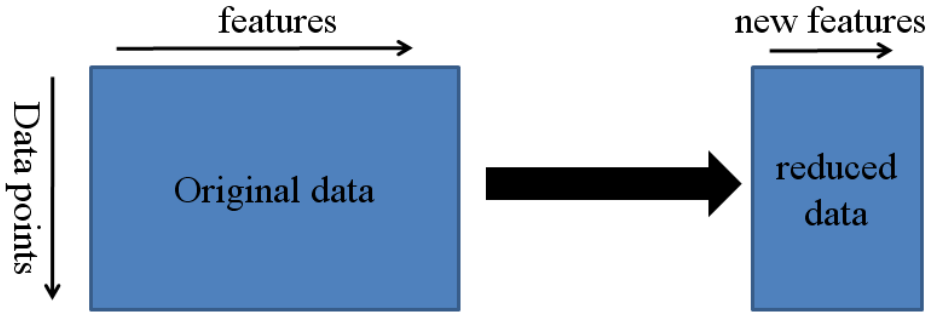
- PCA is commonly applied to datasets to assess information content.
- Example:
  - PCA applied on patient dataset and samples projected on top principal components.
  - Patients with known treatment outcomes are color identified (responders vs non-responders).



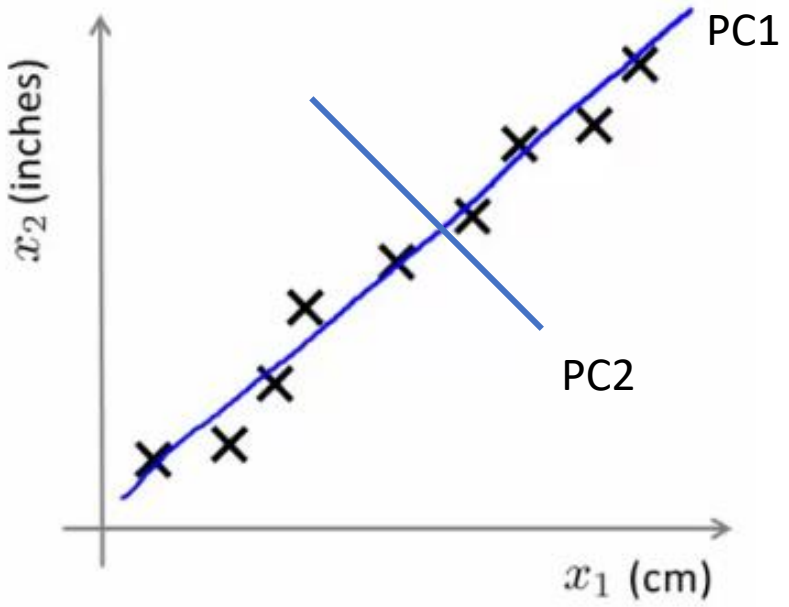
Source: Khodayari-Rostamabad (2011)

Dimensionality Reduction

- Projecting onto principal components can improve model/algorithm performance.
  - Reduces the number of parameters and required complexity



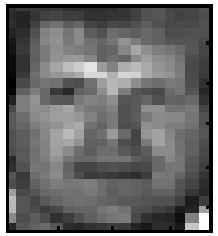
- Example:
  - PC1 captures most of the variance (information).
  - PC2 limited variance and projections onto PC2 would look similar (or the same) for all samples.



What about Images?

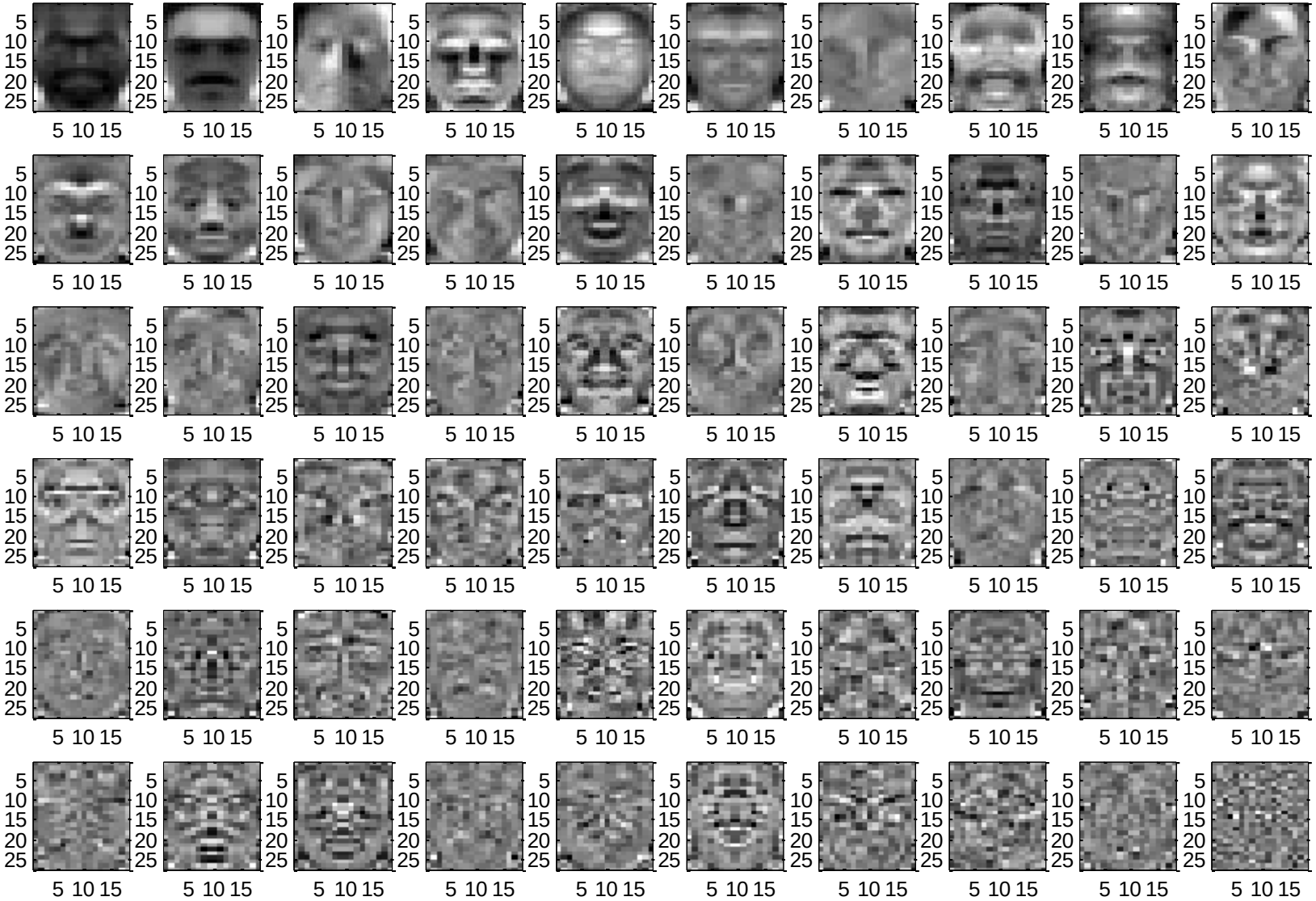
- Images?
  - Yes, we can use PCA! (Turk, Pentland, 1991)

- Each 150 pixel × 150 pixel image can be represented by a 22,500-long vector

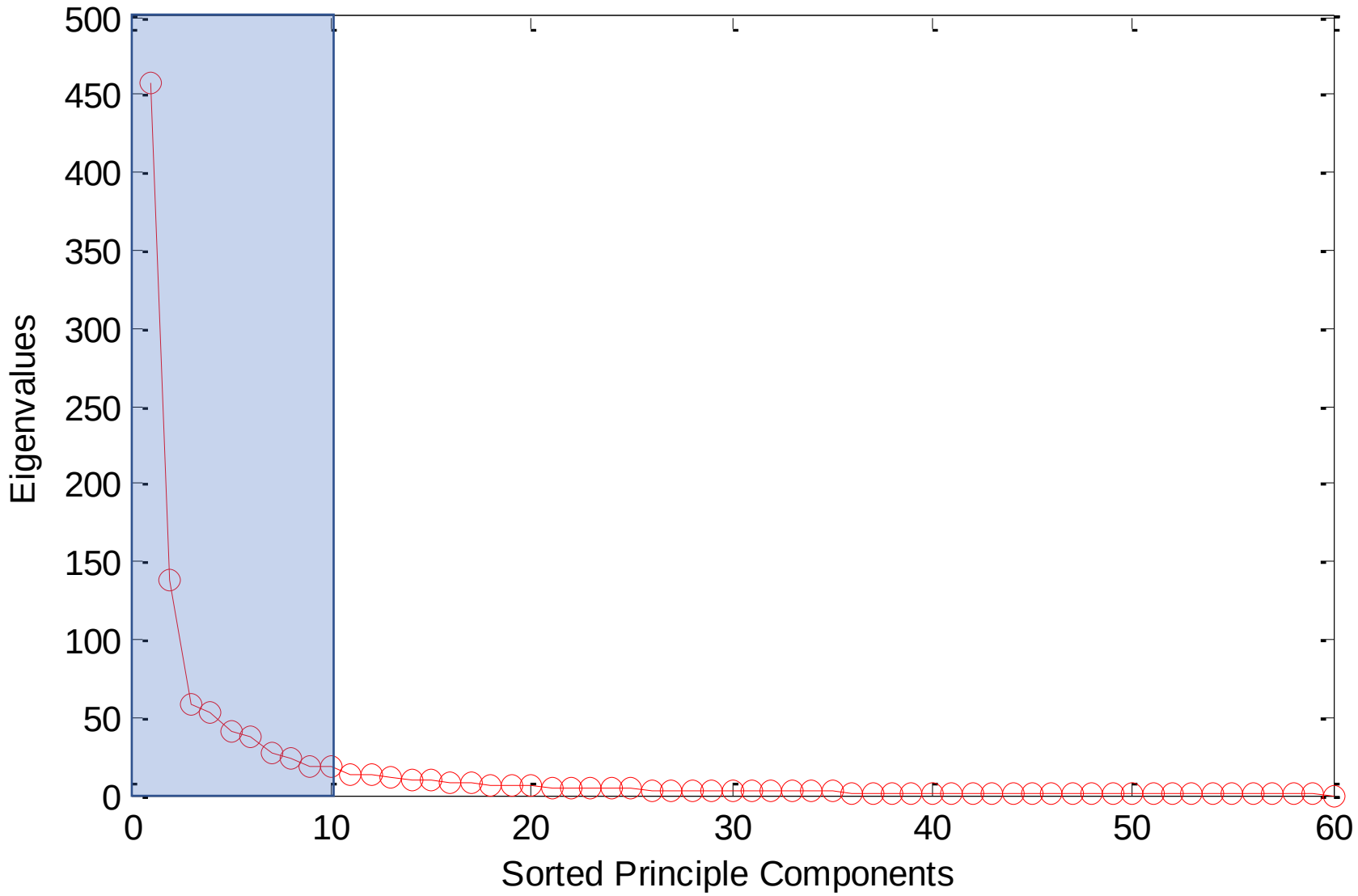


Normalized Face Data

The Eigenfaces

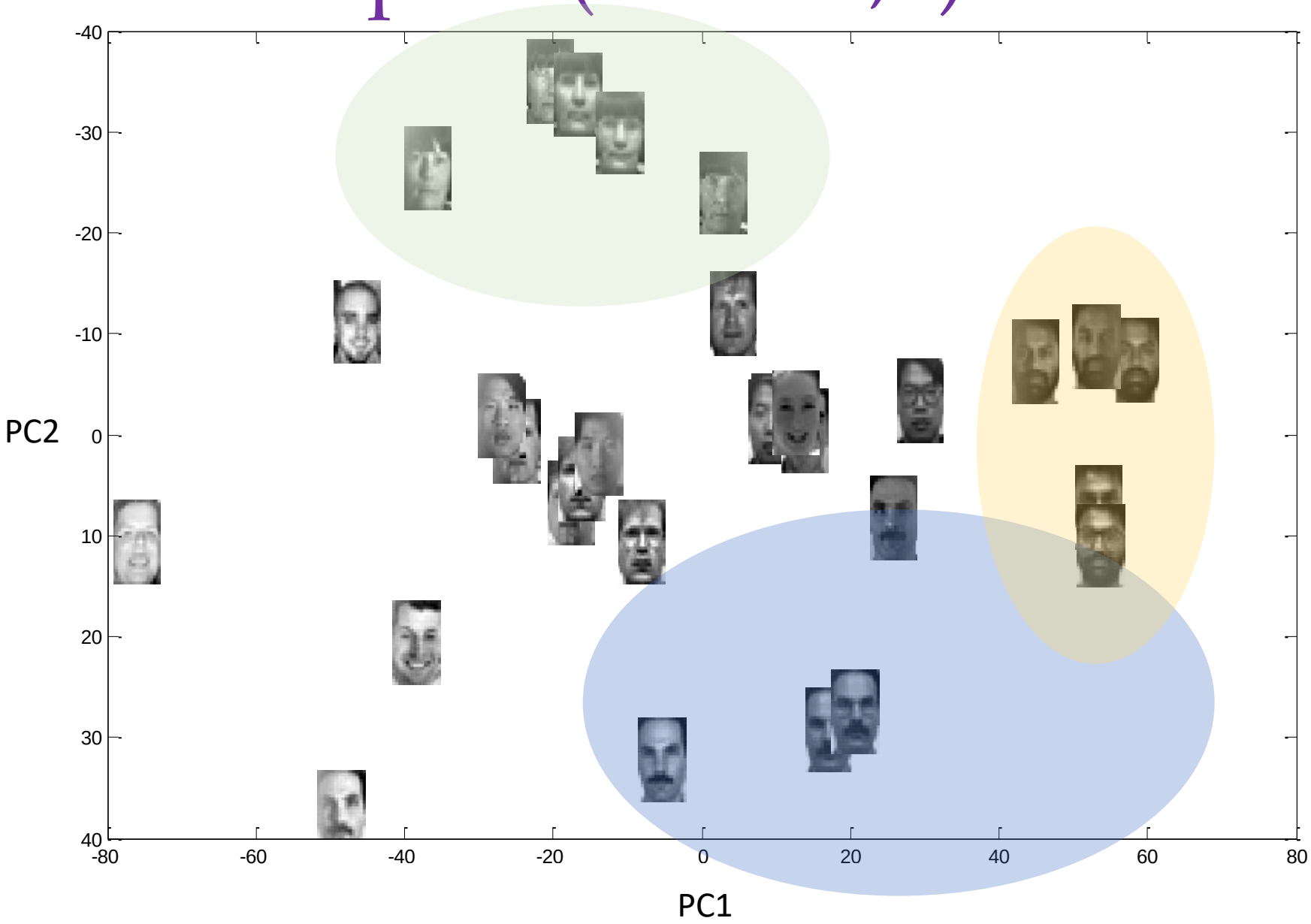


Eigenvalues for each Eigenface



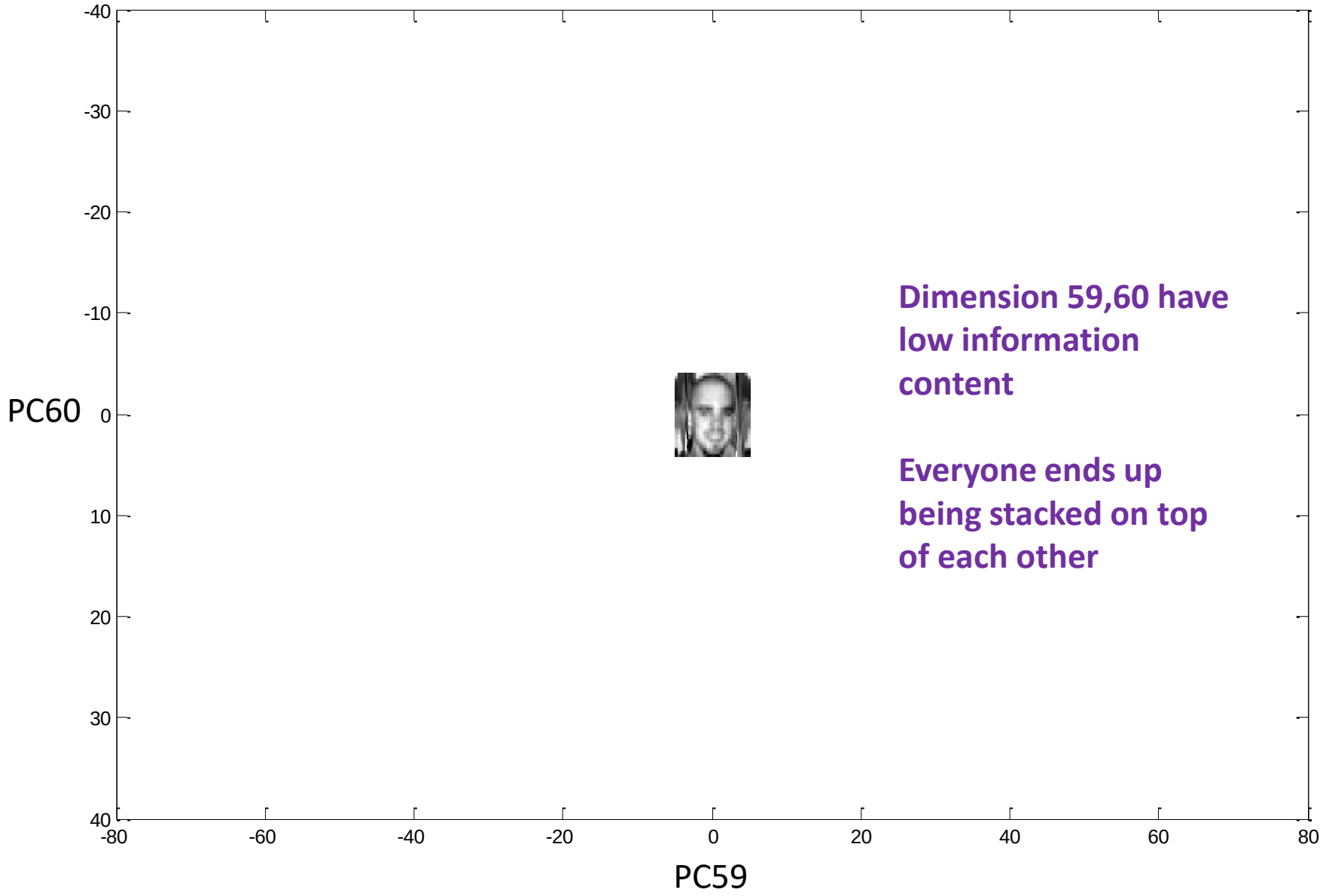
Reconstructing a Face from PCs

Faces in PC-space (Dims 1,2)



Are there any patterns presented?

Faces in PC-space (Dims 59,60)



Data Security

- To reconstruct data we require the mean and standard deviation used for normalization
- Can be used to **secure your datasets** as described for a sample dataset on Kaggle:

> "It contains only numerical input variables which are the result of a PCA transformation. Unfortunately, due to **confidentiality issues, we cannot provide the original features** and more background information about the data. **Features V1, V2, … V28 are the principal components obtained with PCA**, the only features which have not been transformed with PCA are 'Time' and 'Amount'."

Source: Kaggle Credit Card Fraud

Limitations of PCA

- High dimensional data can be problematic. For example, when you have short (small n) and wide data (large p), PCA may not work well.

- We can speed up eigenfaces decomposition by exploiting the smaller dimension of m x n, to do this we need a way to work with rectangular matrices…

Singular Value Decomposition (SVD) to the rescue!

Next Time

- Week 7 Tutorial, Thursday and Friday
  - Project 3 is on PCA and is due 11 March
- Lecture 8 – Dimensionality Reduction Part 2
  - Vector Calculus
  - Singular Value Decomposition (SVD)
  - Interpreting Features
  - Reconstruction
  - Applications
- Guest Lecture on 15 March at 10:00
  - Dr. Sophie Lohmann: “Limits of measurement - who are we measuring?“
  - Zoom link https://utoronto.zoom.us/j/86722516215