SVD, Multivariate Gaussians, Principal Component Analysis (PCA) and Dimensionality Reduction

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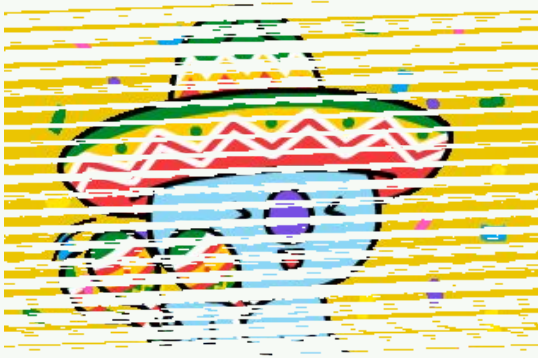
MidTerm Projects

Congratulations on your project

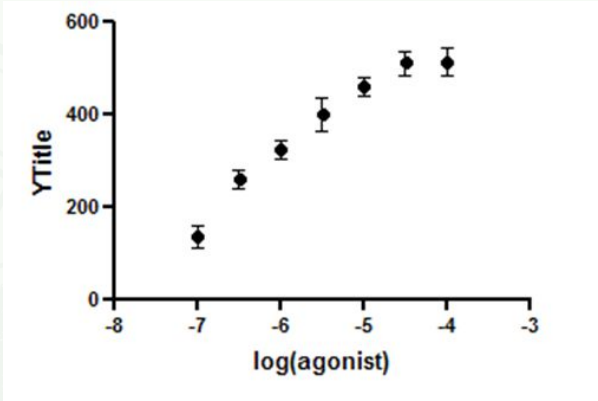


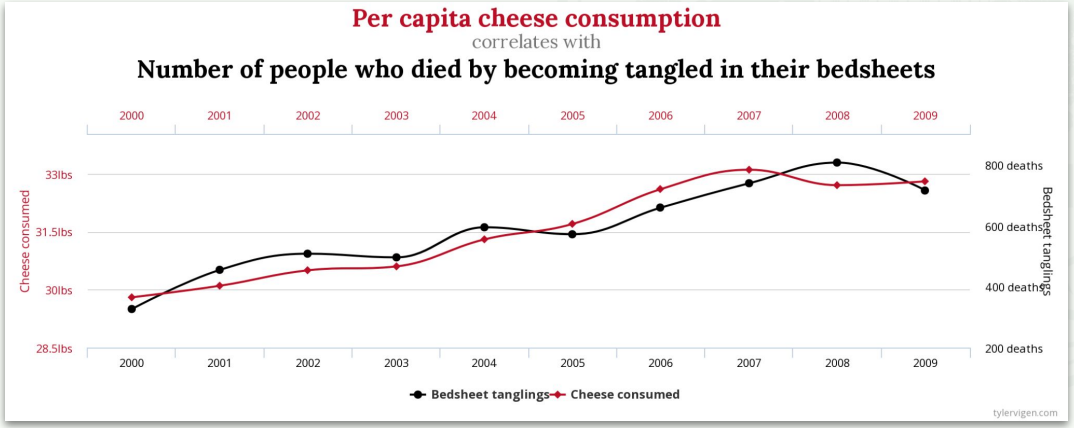
Comments:

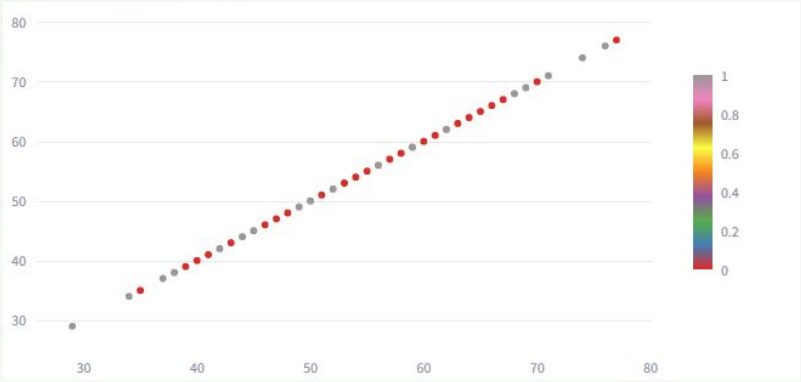
- Project is not assignment, it is a showcase
  - Programming ability
  - Creativity
  - Problem Solving

MidTerm Projects

Visualization is the proof for your project claims, but alone it doesn't carry anything

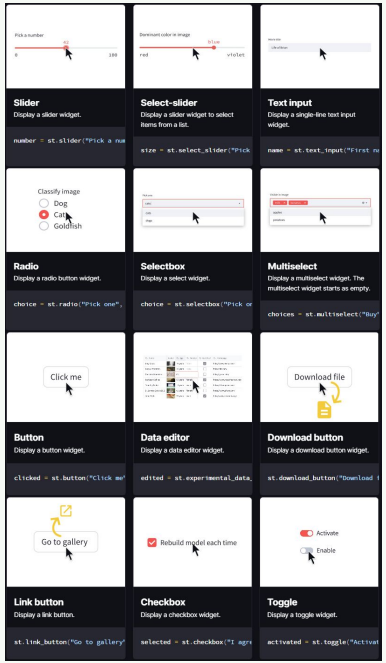




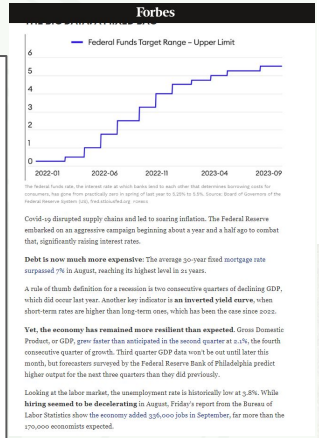


MidTerm Projects

Webapp Design



- Section 1
- Section 2
- Section 3
- Tab 1
- Tab 2
- Tab 3



- The story must make sense
- The option should affect unnecessary materials

Calendar

Lecture and ICA on PCA, SD

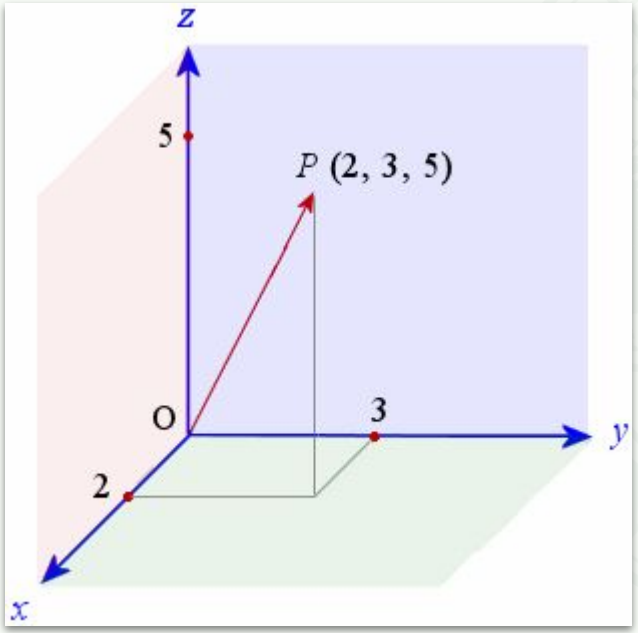
Project Presentation

Project Submission

Class Ends!

Vectors

In engineering and physical sciences, vectors are used to describe quantities that have both a magnitude/size and a direction.



Examples of vectors are:

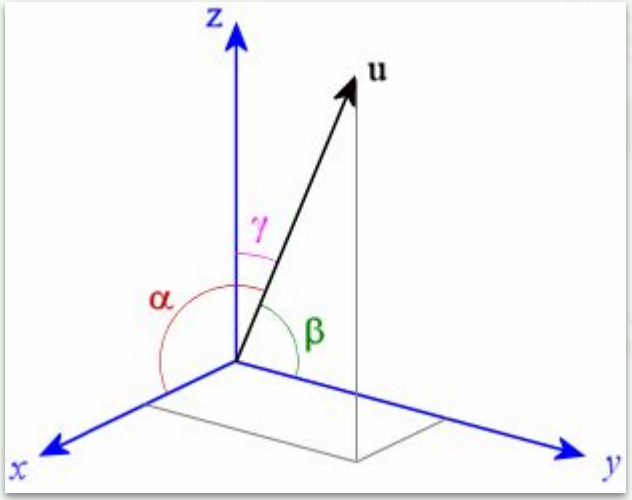
- velocity (which is speed and a direction)
- distance
- force

Vectors have components, usually in our usual 3D physical space.

Dot Products from Vector Analysis

Important for DS, we are interested in the “projection” of the vector on the axes.

This is equivalent to, say, “*what is the x velocity?*”

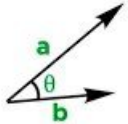


$$\vec{a} = (a_1\vec{i} + a_2\vec{j} + a_3\vec{k})$$

$$\vec{b} = (b_1\vec{i} + b_2\vec{j} + b_3\vec{k})$$

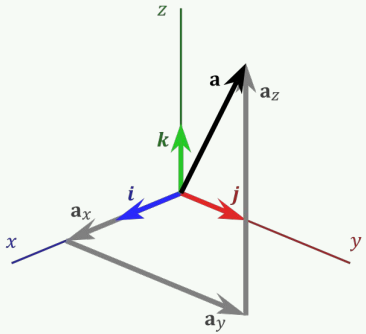
$$\vec{a} \cdot \vec{b} = (a_1\vec{i} + a_2\vec{j} + a_3\vec{k}) \cdot (b_1\vec{i} + b_2\vec{j} + b_3\vec{k})$$

$$= a_1b_1 + a_2b_2 + a_3b_3$$



$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}||\mathbf{b}| \cos\theta$$

$$\cos\theta = \frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a}||\mathbf{b}|}$$



Dot Products are Inner Products

$$\vec{A}^T = \begin{bmatrix} A_1 & A_2 & A_3 \end{bmatrix} \qquad \vec{B} = \begin{bmatrix} B_1 \\ B_2 \\ B_3 \end{bmatrix}$$

$$\begin{bmatrix} A_1 & A_2 & A_3 \end{bmatrix} \begin{bmatrix} B_1 \\ B_2 \\ B_3 \end{bmatrix} = A_1B_1 + A_2B_2 + A_3B_3 = \vec{A}.\vec{B}$$

$$\vec{a} = (a_1\vec{i} + a_2\vec{j} + a_3\vec{k})$$

$$\vec{b} = (b_1\vec{i} + b_2\vec{j} + b_3\vec{k})$$

$$\vec{a} \cdot \vec{b} = (a_1\vec{i} + a_2\vec{j} + a_3\vec{k}) \cdot (b_1\vec{i} + b_2\vec{j} + b_3\vec{k})$$

$$= a_1b_1 + a_2b_2 + a_3b_3$$

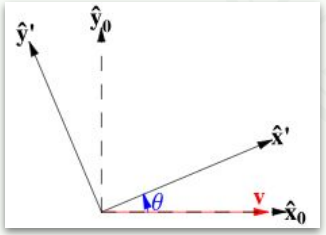
Matrix multiplication can be interpreted as a dot product (or, projection).

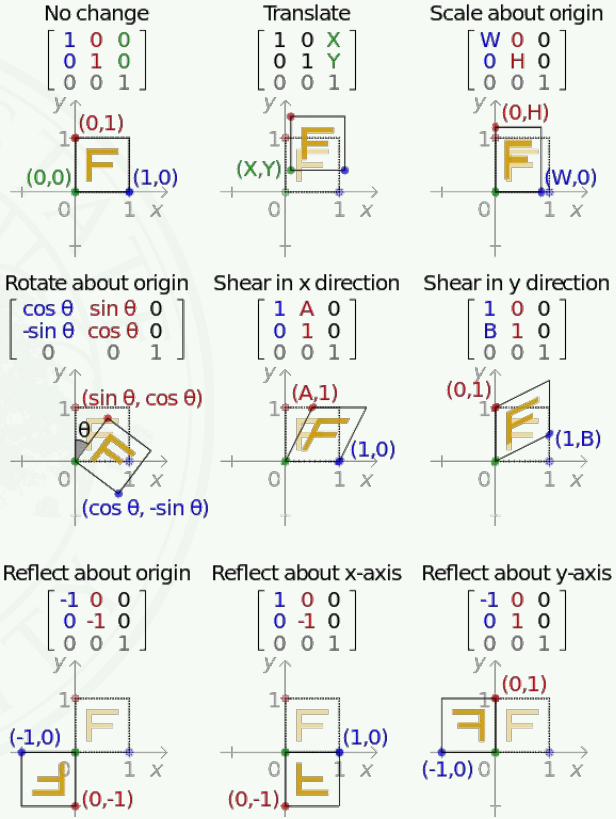
Matrices as Transformations

Matrix multiplication of a vector can be seen as a transformation of that vector to a new vector.

Rotation is just one type of transformation:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{bmatrix} \cdot \begin{bmatrix} x \\ y \end{bmatrix}$$





Diagonalization of a Matrix

Consider a square matrix *A*. We can perform a "similarity transformation" to connect *A* to another matrix *D*.

We will assume that *D* is a diagonal matrix.

- d_i are the "*eigenvalues*"
- p_i are the "*eigenvectors*"

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

$$AP = PD$$

$$\begin{bmatrix} a_{11} & a_{12} & \dots \\ a_{21} & a_{22} & \dots \\ \vdots & \vdots & \dots \end{bmatrix} \begin{bmatrix} | & | & \dots \\ p_1 & p_2 & \dots \\ | & | & \dots \end{bmatrix} = \begin{bmatrix} | & | & \dots \\ p_1 & p_2 & \dots \\ | & | & \dots \end{bmatrix} \begin{bmatrix} d_1 & 0 & \dots \\ 0 & d_2 & \dots \\ \vdots & \vdots & \dots \end{bmatrix}$$

$$Ap_i = d_i p_i$$ stretch a vector with no rotation

Diagonalization As a Change of Basis

1. *A* transforms ***x*** into ***y***

$$A\mathbf{x} = \mathbf{y}$$

2. solve for *x*, given *A* and ***y***

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

$$PDP^{-1}\mathbf{x} = \mathbf{y}$$

$$DP^{-1}\mathbf{x} = P^{-1}\mathbf{y}$$

original data projected onto eigenvalues

components act independently in new basis

$$D\mathbf{x}' = \mathbf{y}'$$

$$\mathbf{x}' = D^{-1}\mathbf{y}'$$

$$\mathbf{x} = PD^{-1}P^{-1}\mathbf{y}$$

Statistical Properties of the Data Matrix *X*

We have explored statistics a bit earlier in the course.

Let's connect the statistical properties of the data to newer ideas, such as the SVD.

Remove Mean From Data Matrix

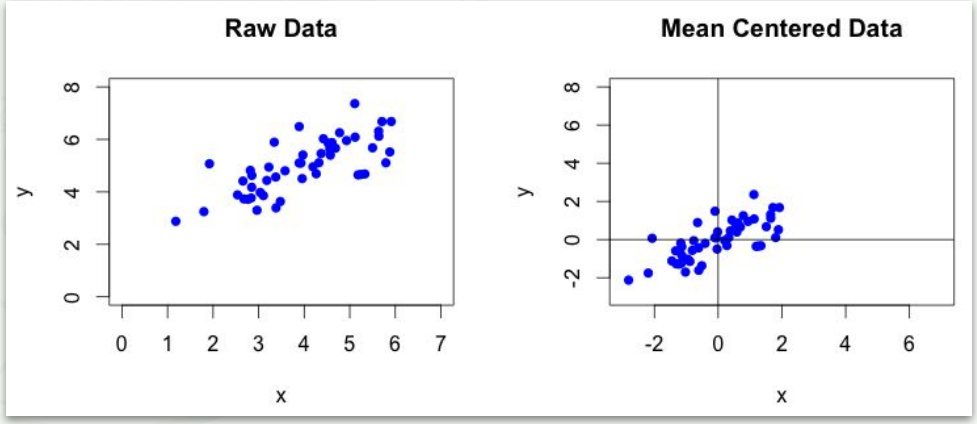
features

$$X = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \end{bmatrix}$$

samples

μ_1 μ_2

$$X' = \begin{bmatrix} x_{11} - \mu_1 & x_{12} - \mu_2 \\ x_{21} - \mu_1 & x_{22} - \mu_2 \\ x_{31} - \mu_1 & x_{32} - \mu_2 \end{bmatrix}$$



Covariance Reminder

$$
\begin{aligned}
\operatorname{cov}(X, Y) &= \mathrm{E}[(X - \mathrm{E}[X])\,(Y - \mathrm{E}[Y])] \\
&= \mathrm{E}[XY - X\,\mathrm{E}[Y] - \mathrm{E}[X]Y + \mathrm{E}[X]\,\mathrm{E}[Y]] \\
&= \mathrm{E}[XY] - \mathrm{E}[X]\,\mathrm{E}[Y] - \mathrm{E}[X]\,\mathrm{E}[Y] + \mathrm{E}[X]\,\mathrm{E}[Y] \\
&= \mathrm{E}[XY] - \mathrm{E}[X]\,\mathrm{E}[Y],
\end{aligned}
$$

Variance and Covariance

Here, *X* is mean centered.

Recall that the covariance is defined in terms of centered data.

$$C = \frac{X^T X}{n-1},$$

$$\begin{bmatrix} \text{Var}(x_1) & \cdots\cdots & \text{Cov}(x_n, x_1) \\ \vdots & \cdot & \vdots \\ \vdots & \cdot & \vdots \\ \text{Cov}(x_n, x_1) & \cdots\cdots & \text{Var}(x_n) \end{bmatrix}$$

Let's use the smallest non-trivial data matrix.

$$X = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \end{bmatrix}$$

$$X^T X = \begin{bmatrix} x_{11} & x_{21} & x_{31} \\ x_{12} & x_{22} & x_{32} \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \end{bmatrix},$$

$$= \begin{bmatrix} x_{11}^2 + x_{21}^2 + x_{31}^2 & x_{11}x_{12} + x_{21}x_{22} + x_{31}x_{32} \\ x_{12}x_{11} + x_{22}x_{21} + x_{32}x_{31} & x_{12}^2 + x_{22}^2 + x_{32}^2 \end{bmatrix}$$

Note on Normalization and Choice of Transpose

You don't always see this definition.

You might also see:

- no factor of *n-1*,
- a factor of *n* instead,
- transpose might be reversed.

$$C = \frac{X^T X}{n-1},$$

$$C_1 = X^T X$$

$$C_2 = X X^T$$

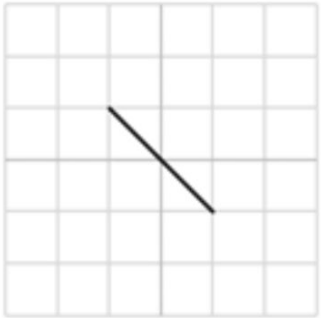
Note that these C are square, but have different meanings.

Geometric Interpretation I

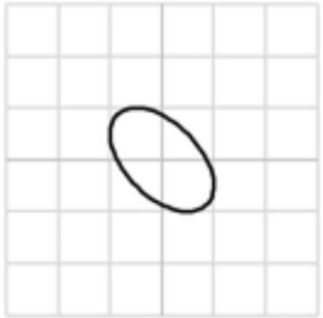
Correlation matrix

Correlation matrix has 1 in diagonals and values betwen -1 and 1 inclusive in off-diagonals. Ellipse size remains the same (always touches square of side 2 units). Whether the correlation is positive or negative can be observed by the orientation of the ellipse. The amount of correlation can be interpreted by how thin the ellipse is.

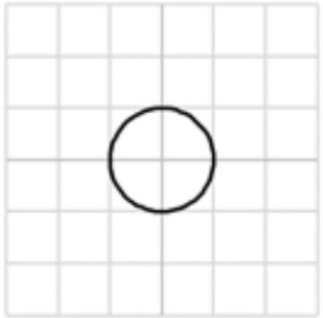
$$\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$



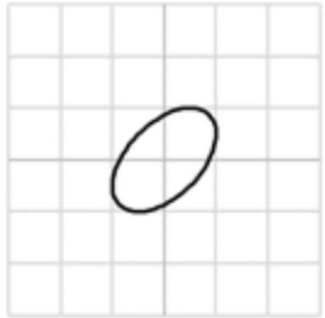
$$\begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}$$



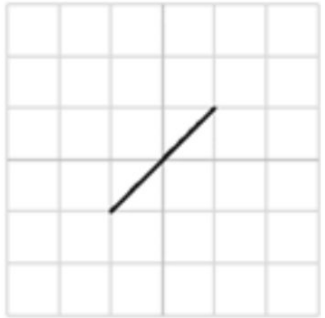
$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$



$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

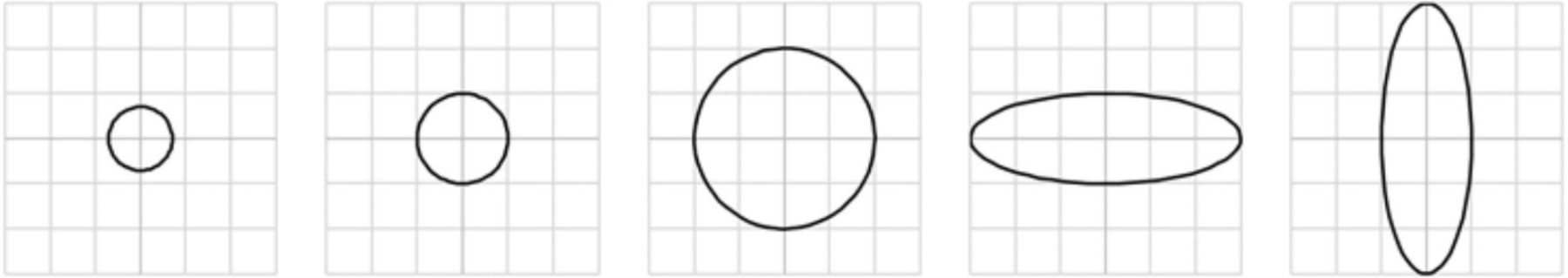


Geometric Interpretation II

Diagonal matrix

Zeros in off-diagonals means zero correlation. Ellipse axes are parallel to coordinate axes (no rotation).

$\begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$ $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ $\begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix}$ $\begin{bmatrix} 9 & 0 \\ 0 & 1 \end{bmatrix}$ $\begin{bmatrix} 1 & 0 \\ 0 & 9 \end{bmatrix}$

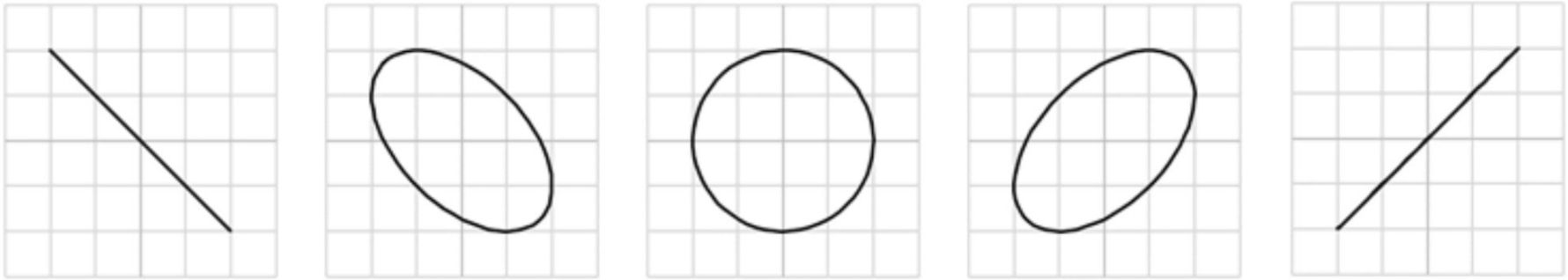


Geometric Interpretation III

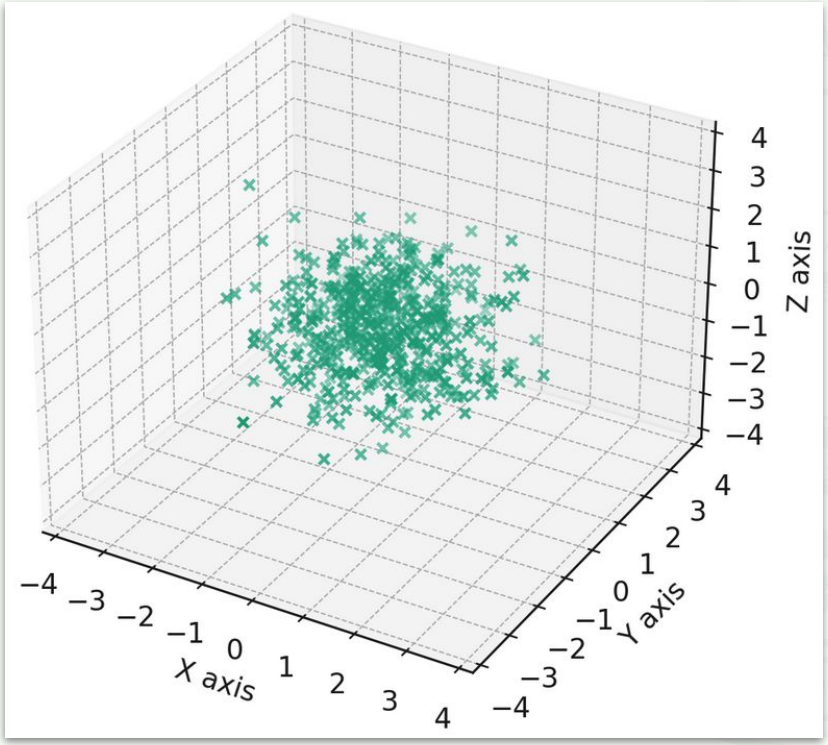
Same values in diagonals

Ellipse is rotated 45 degrees if correlation (off-diagonal) is positive regardless of its magnitude. Similarly -45 degrees if correlation is negative.

$\begin{bmatrix} 4 & -4 \\ -4 & 4 \end{bmatrix}$ $\begin{bmatrix} 4 & -2 \\ -2 & 4 \end{bmatrix}$ $\begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix}$ $\begin{bmatrix} 4 & 2 \\ 2 & 4 \end{bmatrix}$ $\begin{bmatrix} 4 & 4 \\ 4 & 4 \end{bmatrix}$



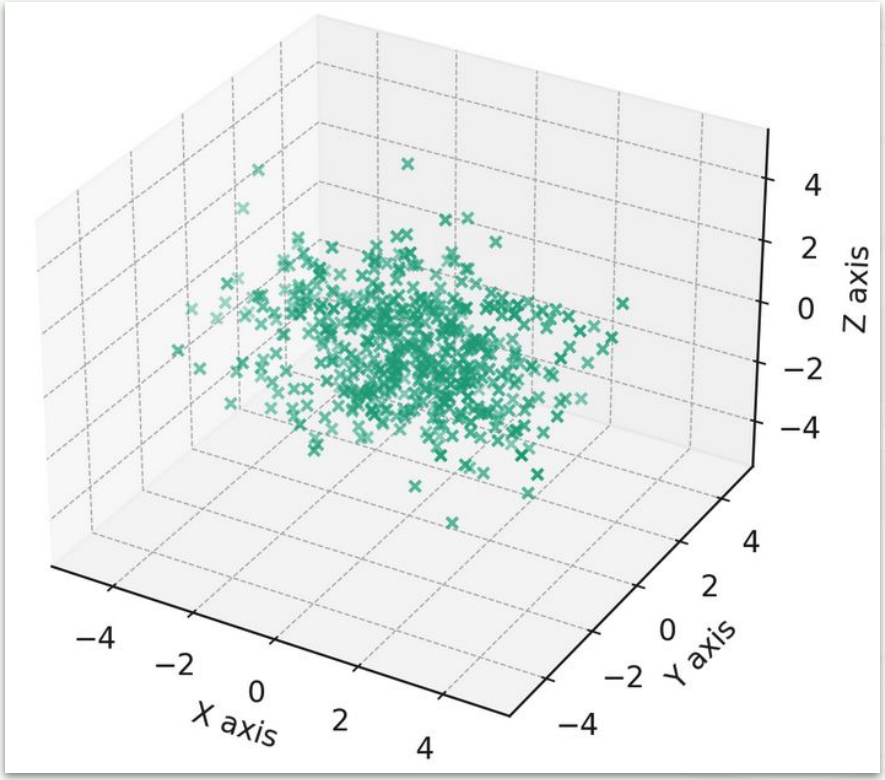
Let’s examine some data sets!



covariance matrix

$$\begin{pmatrix} 0.996 & -0.039 & 0.028 \\ -0.039 & 0.998 & -0.098 \\ 0.028 & -0.098 & 0.982 \end{pmatrix}$$

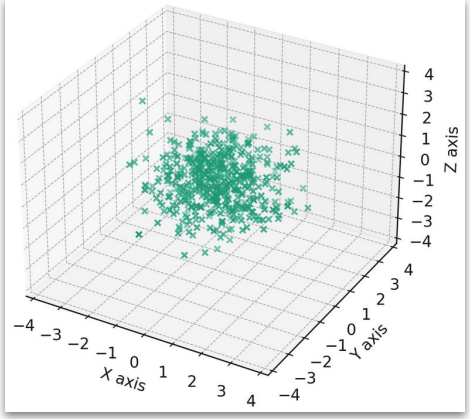
Let’s examine some data sets!



covariance matrix

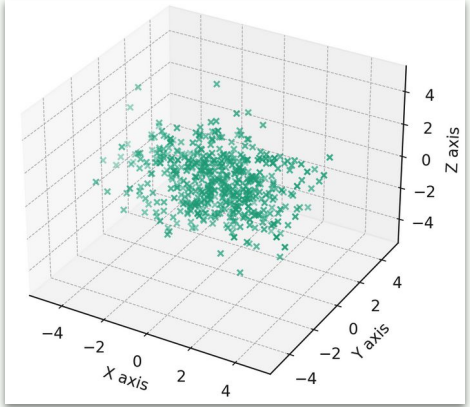
$$\begin{pmatrix} 3.204 & 0.113 & -0.046 \\ 0.113 & 0.911 & 0.092 \\ -0.046 & 0.092 & 1.976 \end{pmatrix}$$

Let's examine some data sets!



$$\begin{pmatrix} 0.996 & -0.039 & 0.028 \\ -0.039 & 0.998 & -0.098 \\ 0.028 & -0.098 & 0.982 \end{pmatrix}$$

Note that these covariance matrices are already (approximately) diagonal.

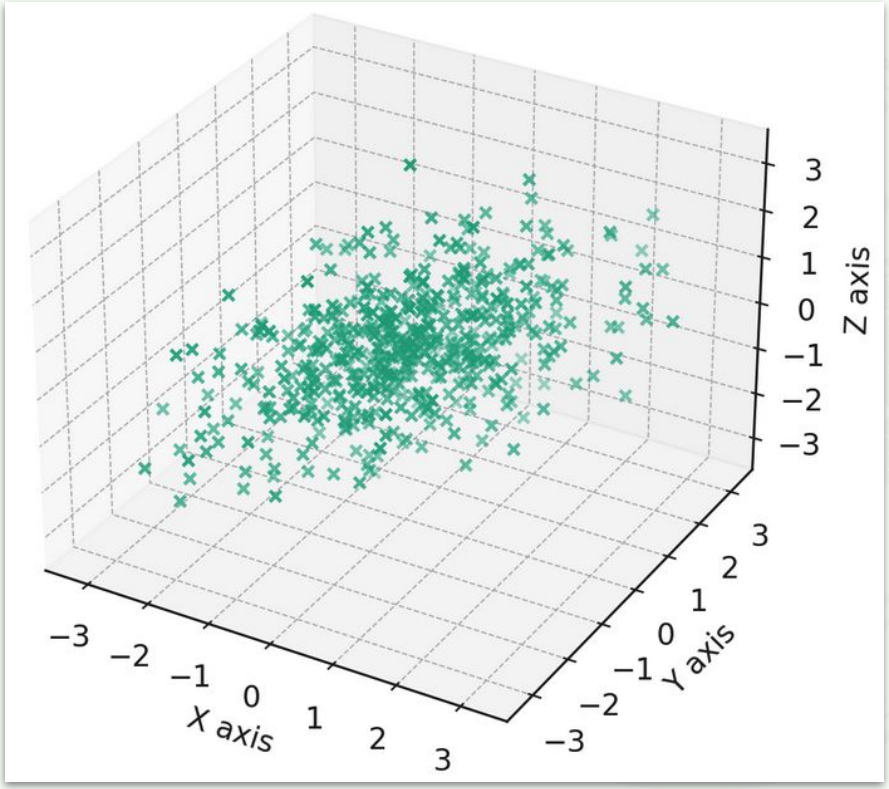


$$\begin{pmatrix} 3.204 & 0.113 & -0.046 \\ 0.113 & 0.911 & 0.092 \\ -0.046 & 0.092 & 1.976 \end{pmatrix}$$

$$f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^k \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

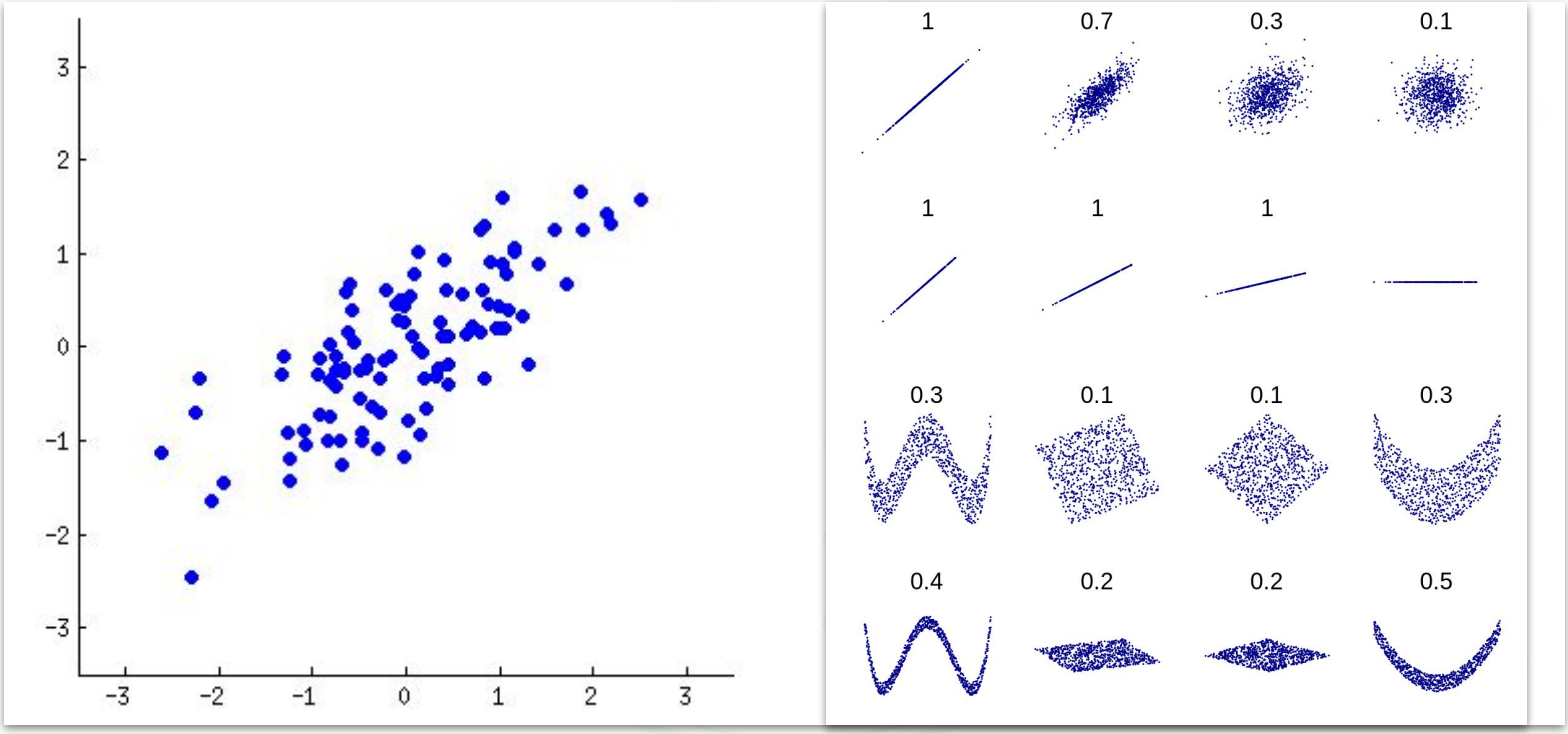
covariance matrix

Non-Diagonal Case



$$\begin{pmatrix} 1.052 & 0.821 & 0.262 \\ 0.821 & 0.958 & 0.461 \\ 0.262 & 0.461 & 0.979 \end{pmatrix}$$

Diagonalizing the Covariance Matrix: Why?



Diagonalizing the Covariance Matrix: Math

$$\mathcal{C} = X^T X$$

$$= PDP^{-1}$$

$$P^{-1}\mathcal{C}P = D$$

$$P^{-1}X^T XP = D$$

$$P^T X^T XP = (XP)^T XP$$

SVD of Covariance Matrix

$$
\begin{aligned}
X^T X &= (U\Sigma V^T)^T U\Sigma V^T, \\
&= V\Sigma^T U^T U\Sigma V^T, \\
&= V\Sigma^T \Sigma V^T, \\
&= V\Sigma^2 V^T, \\
&= V\Lambda V^T,
\end{aligned}
$$

Note the importance of the matrix *V* in the covariance.

When we write a matrix in this form, we say we have “diagonalized” the matrix.

The diagonal matrix Λ contains the eigenvalues, which are the squares of the singular values.

Expand Correlation in Singular Values (SVs)

$$C = X^T X$$

$$= V \Lambda V^T$$

$$= \sum_i \lambda_i v_i v_i^T$$

$$\lambda_i = \sigma_i^2$$

Each vector in V “explains” some of the variance in the dataset.

The first column of V contributes the most because it is associated with the largest SV in the sum.

New Coordinate System: Project Onto *V*

How can we understand this result?

$$X^T X = V \Sigma^2 V^T,$$

$$V^T X^T X V = \Sigma^2,$$

$$(XV)^T XV = \Sigma^2,$$

$$(Y)^T Y = \Sigma^2$$

PCA: Columns of *V*

The columns of *V* are called the "*principal components*" (directions) of *X*.

The first principal component of *X* is: Xv_1

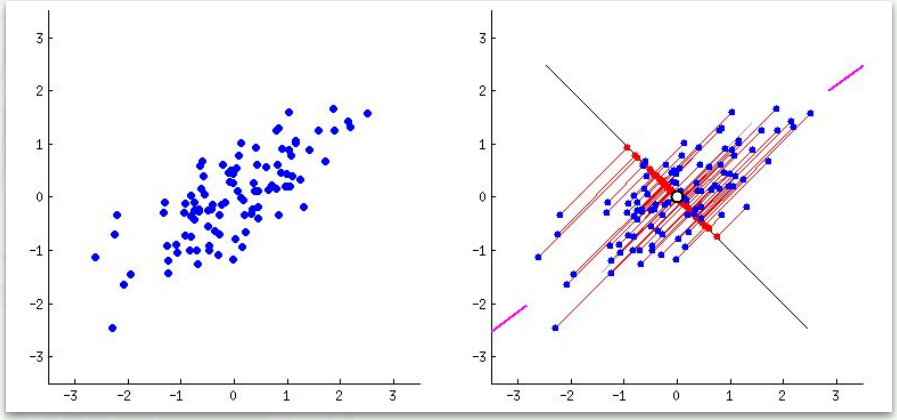
The variance of the first principal component of *X* is: $\mathrm{Var}(Xv_1) = \frac{\sigma_1^2}{n-1}$

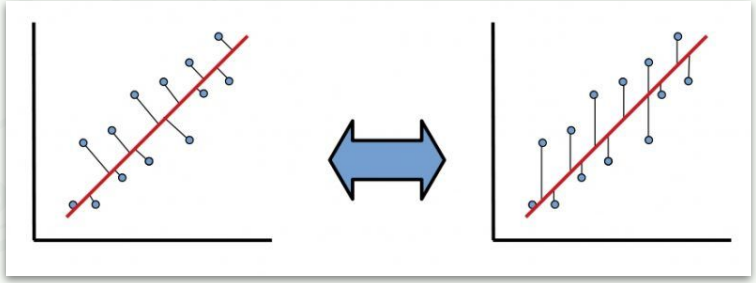
Principal Component Analysis (PCA)

Given a dataset, the principal components are vectors v_i that best describe the variance in the data.

The vectors are orthogonal to each other.

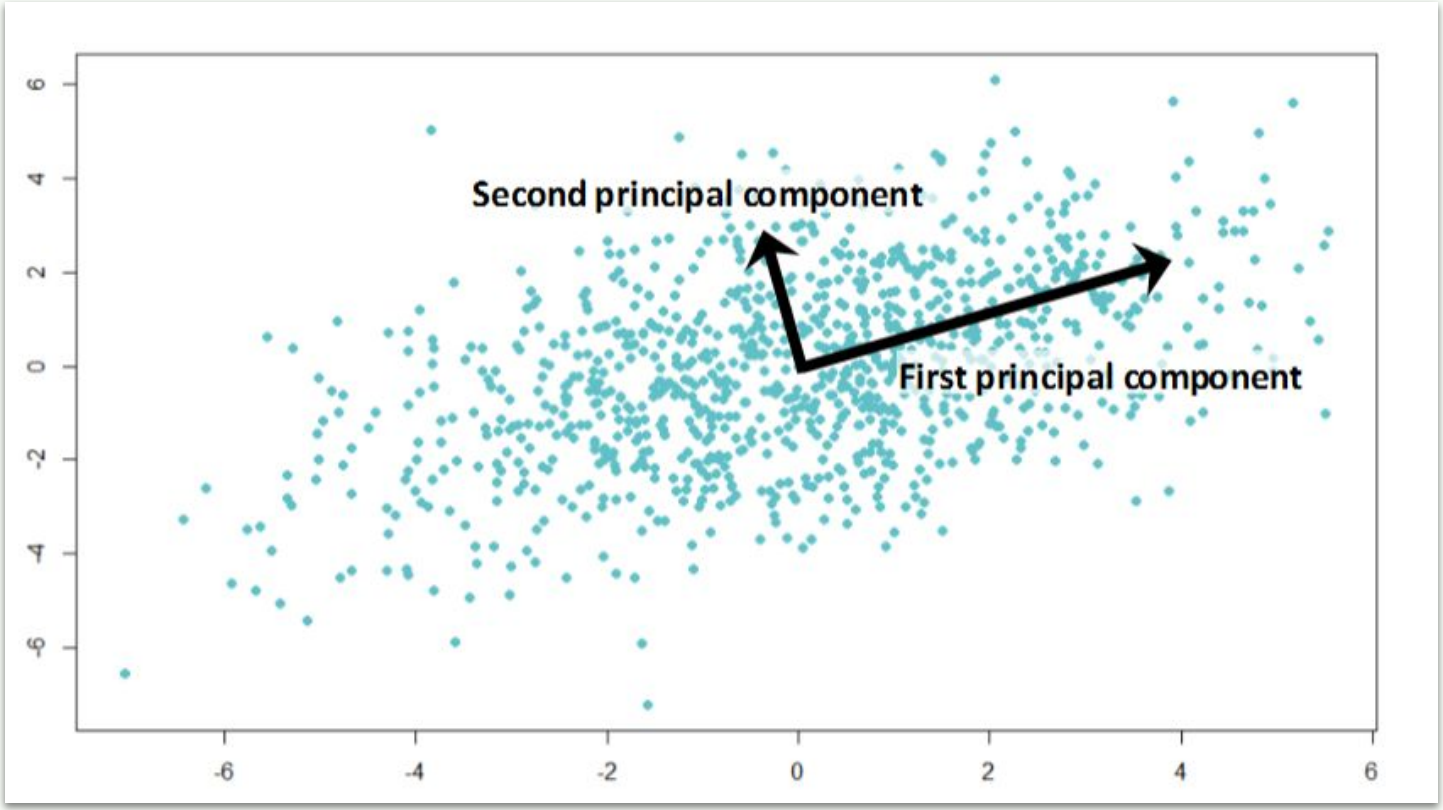
The "best fit" is defined by minimizing the *perpendicular* distance of the data to the line(s).



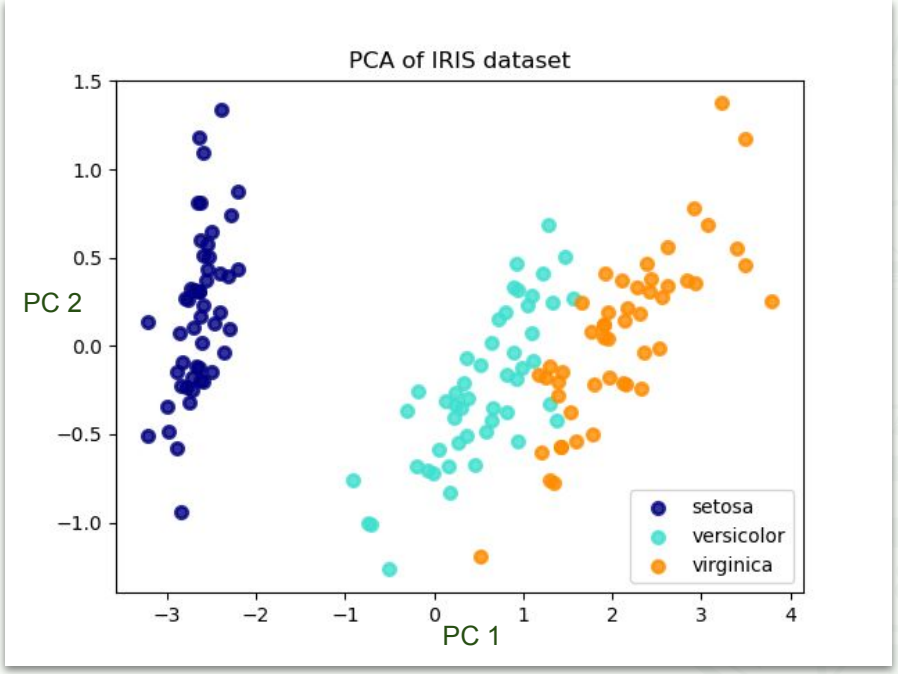


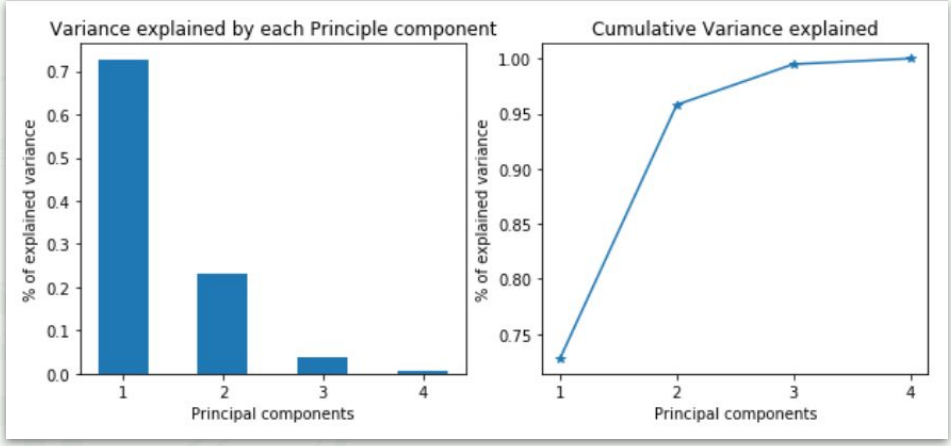
Don't confuse the best fit line in PCA with a line used for modeling.

PCA Vectors


Second principal component
First principal component
6
4
2
0
-2
-4
-6
-6
-4
-2
0
2
4
6

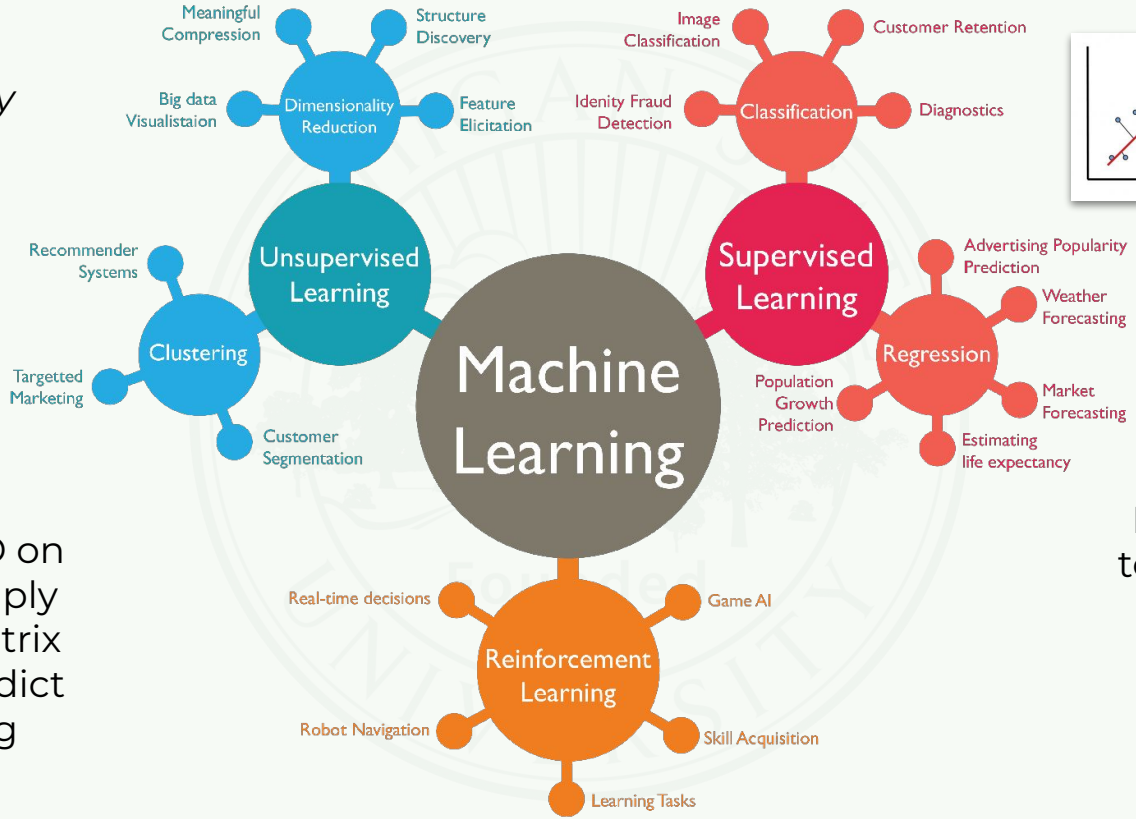
Iris Example

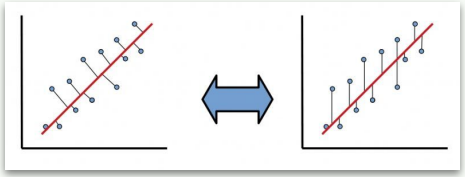




Organization of Machine Learning

There is no known *y* in unsupervised learning.



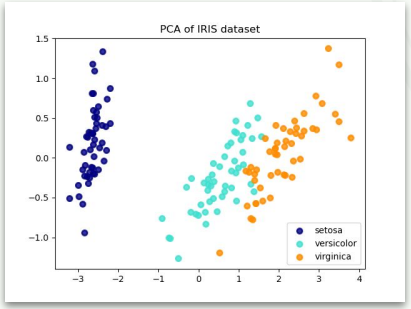


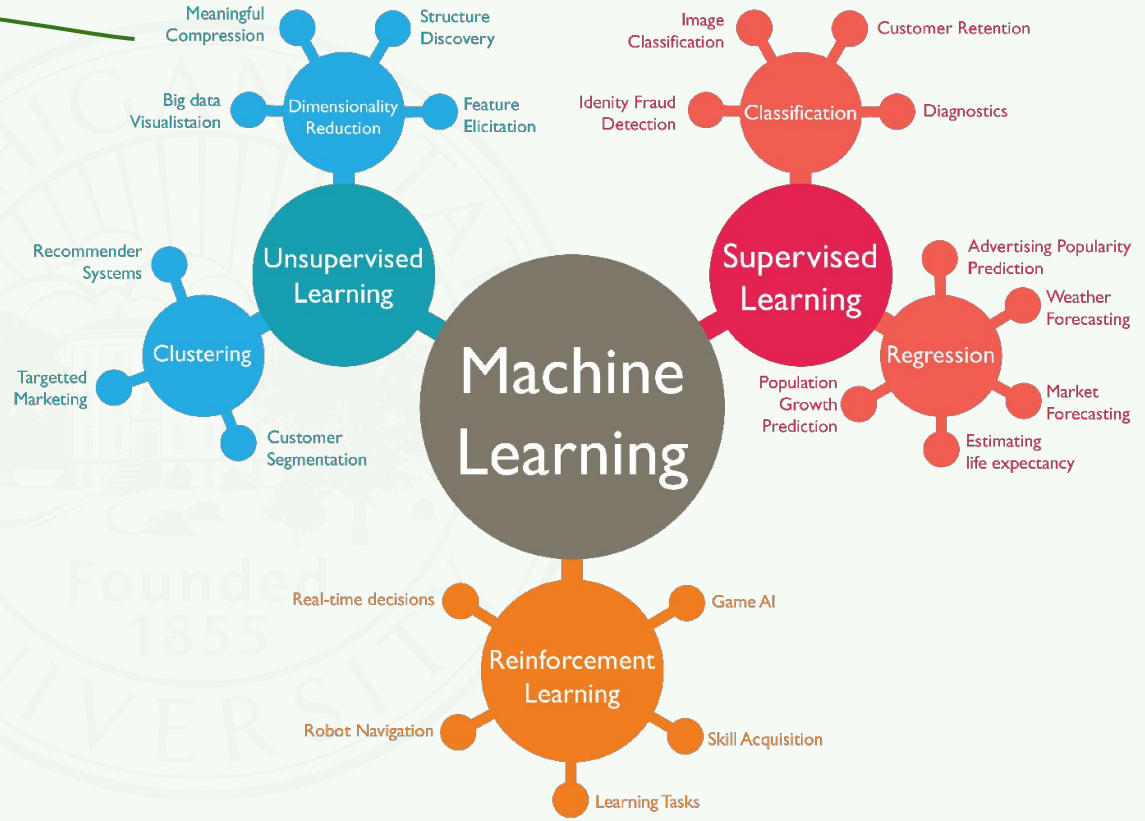
When we did SVD on an image, we simply used the data matrix *X* with no *y* to predict or use in finding weights.

Regression is used to predict a *y* (indep var) in terms of many *x* (dep vars).

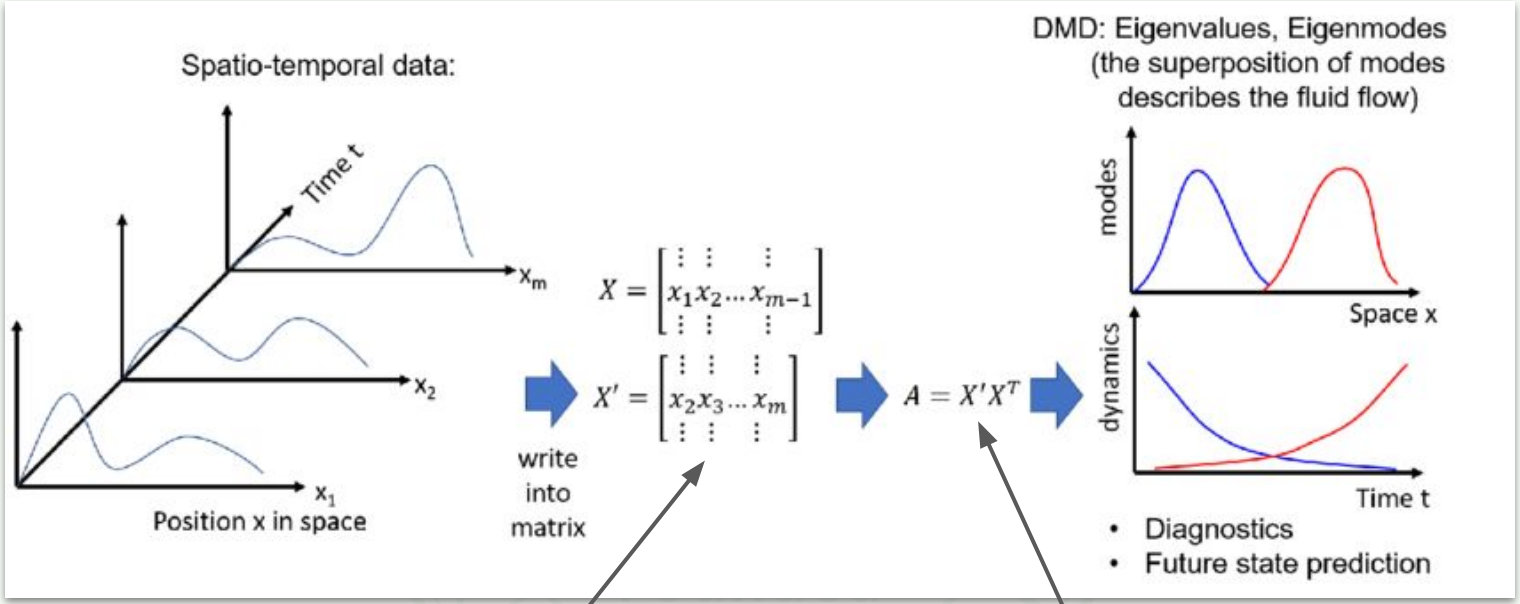
Dimensionality Reduction

dimensionality reduction: transform data to a lower-dimensional space that preserves important features of the data





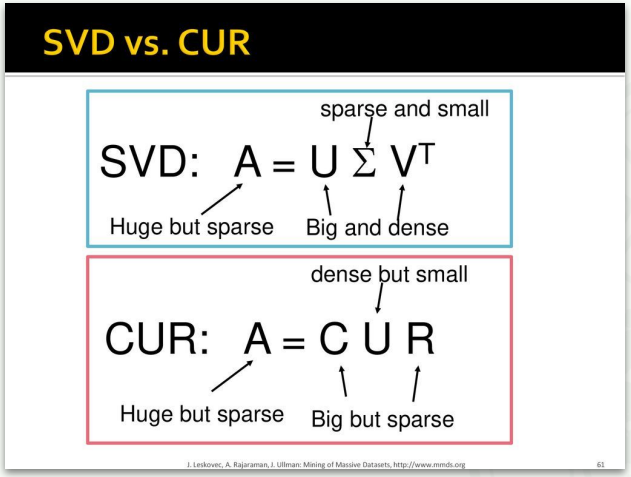
Note on Spatiotemporal Data

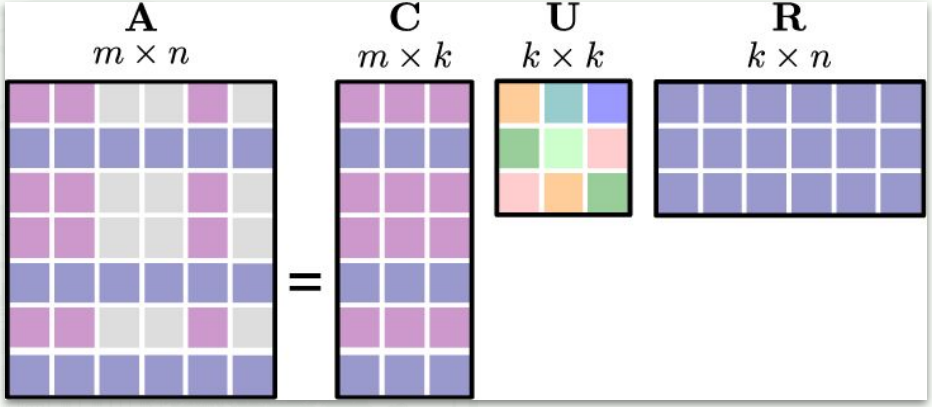


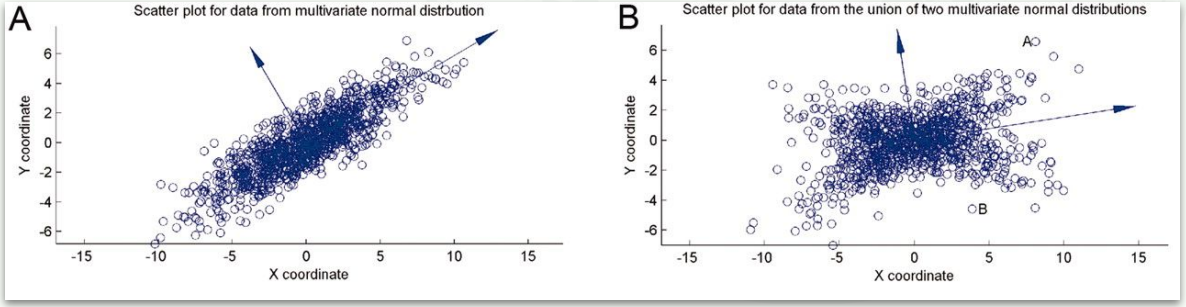
In this case, the values in each column are not different data samples, but values at specific spatial points. X^TX and XX^T have important physical meanings: averages over space and time.

For time dependent data we can form generalizations of the correlation matrix that includes changes over time. That correlation matrix contains interesting information about the dynamics.

SVD/PCA Are Common, But Not Always Best







PCA is based on covariance, which may not best capture the structure in the data.