

# APS1070

Foundations of Data Analytics and  
Machine Learning

Winter 2022

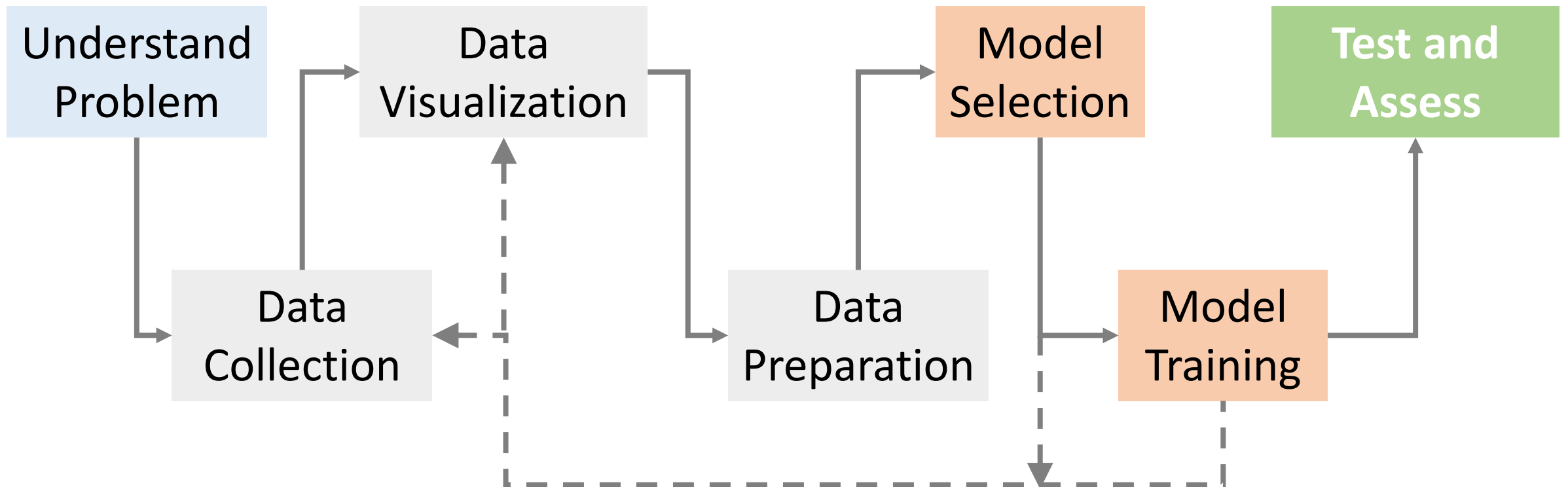
## **Week 8:**

- *Singular Value Decomposition (SVD)*
- *Applications*
- *Vector Calculus*

Sinisa Colic and Samin Aref



# Course Theme



# Slide Attribution

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

- Marc Deisenroth
- Jason Riordon

# Last Time

- Looked into PCA for dimensionality reduction
  - Determinant
  - Trace
  - Eigendecomposition
  - PCA Applications
- Today we will introduce SVD for dimensionality reduction and interpretation of data.

# Rectangular Matrices

- Eigendecomposition (and PCA) is **limited to square matrices**
- Q: How then can we perform matrix decomposition on rectangular matrices?

# Motivation: Movie Recommendations

- SVD can also be used to find structure in data for making recommendations on movies.
- More on this later...

	Ali	Beatrix	Chandra	
Star Wars	5	4	1	Sci-fi
Blade Runner	5	5	0	
Amelie	0	0	5	French
Delicatessen	1	0	4	

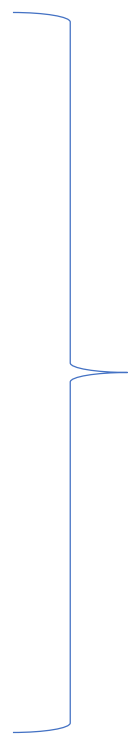
$$= \begin{bmatrix} -0.6710 & 0.0236 & 0.4647 & -0.5774 \\ -0.7197 & 0.2054 & -0.4759 & 0.4619 \\ -0.0939 & -0.7705 & -0.5268 & -0.3464 \\ -0.1515 & -0.6030 & 0.5293 & -0.5774 \end{bmatrix}$$

$$\begin{bmatrix} 9.6438 & 0 & 0 \\ 0 & 6.3639 & 0 \\ 0 & 0 & 0.7056 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} -0.7367 & -0.6515 & -0.1811 \\ 0.0852 & 0.1762 & -0.9807 \\ 0.6708 & -0.7379 & -0.0743 \end{bmatrix}$$

# Agenda

- Recap from last time
  - Eigendecomposition
  - PCA
- SVD
  - SVD vs Eigendecomposition
  - Dimensionality Reduction
  - Interpretations
- Applications
- Vector Calculus
  - Matrix Differentiation



Theme:  
**Dimensionality Reduction  
and Interpretations**

# Matrix Decompositions Continued

Readings:

- MML Chapter 4.5-8



# Recap: Matrix Decomposition

- ☐ Eigenvectors
- ☐ Eigenvalues
- ☐ Determinants
- ☐ Eigendecomposition
- ☐ PCA

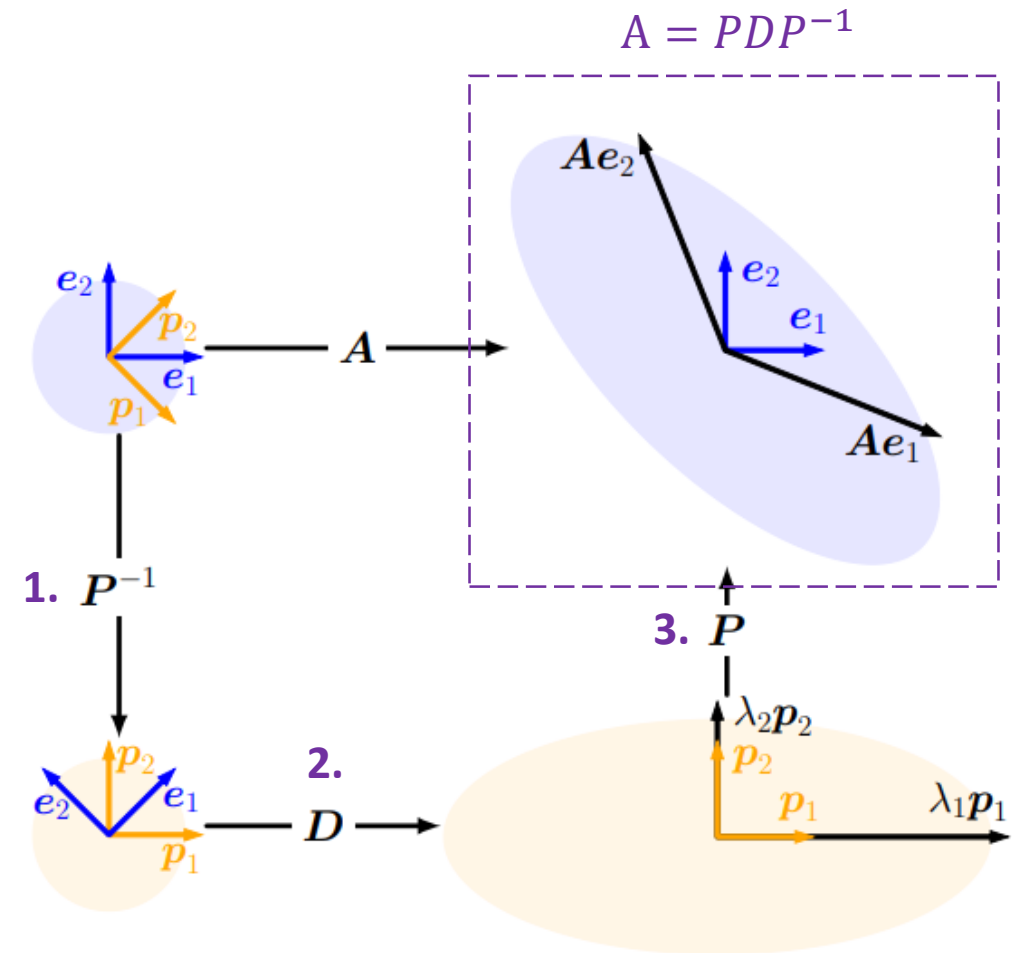
# Recap: Eigendecomposition

- A **square matrix** ( $n \times n$ ) can be factored into:

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

- If the square **matrix** is also **symmetrical** then the eigenvectors will also be orthonormal:

$$A = PDP^T$$



# Recap: Principal Component Analysis

Data Matrix (rectangular)

	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



Covariance Matrix (square)

	feature 2	
feature 1	val1	val2
	val2	val4

- Taking the square (and symmetrical) covariance matrix we obtain:

$$A = PDP^T \quad \text{Spectral Theorem}$$

- To obtain principal components and associated scores:

$$\begin{array}{c}
 \begin{array}{|c|} \hline A \\ \hline \end{array} \\
 \begin{array}{|c|} \hline m \times m \\ \hline \end{array}
 \end{array}
 =
 \begin{array}{c}
 \begin{array}{|c|} \hline Q \\ \hline \end{array} \\
 \begin{array}{|c|} \hline m \times m \\ \hline \end{array} \\
 \downarrow \\
 \text{eigenvector matrix}
 \end{array}
 \times
 \begin{array}{c}
 \begin{array}{|c|} \hline \Lambda \\ \hline \end{array} \\
 \begin{array}{|c|} \hline m \times m \\ \hline \end{array} \\
 \downarrow \\
 \text{eigenvalue matrix}
 \end{array}
 \times
 \begin{array}{c}
 \begin{array}{|c|} \hline Q^T \\ \hline \end{array} \\
 \begin{array}{|c|} \hline m \times m \\ \hline \end{array}
 \end{array}$$

Diagram illustrating the decomposition of the covariance matrix  $A$  into the eigenvector matrix  $Q$ , the eigenvalue matrix  $\Lambda$ , and the transpose of the eigenvector matrix  $Q^T$ . The matrices are shown as grids with dimensions  $m \times m$  indicated below them. Arrows point from the  $Q$  and  $\Lambda$  matrices to their respective labels: "eigenvector matrix" and "eigenvalue matrix".

# Recap: Matrix Decomposition

- We would like a general approach for **decomposing rectangular matrices**.
- PCA is already applied to rectangular matrices...
- Mathematically PCA is:

$$A = XX^T = PDP^T$$

when the mean/expectation across each variable/feature is zero

# Singular Value Decomposition

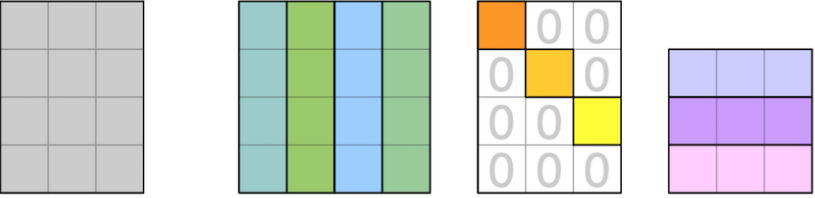
- We would like to obtain the following decomposition for a **rectangular matrix**:

$$A = U\Sigma V^T$$

The diagram shows the dimensions of the matrices in the SVD equation  $A = U\Sigma V^T$ . Matrix  $A$  is represented by a rectangle with height  $m$  and width  $n$ . Matrix  $U$  is a square with side length  $m$ . Matrix  $\Sigma$  is a rectangle with height  $m$  and width  $n$ . Matrix  $V^T$  is a square with side length  $n$ . The equation is shown as  $A = U\Sigma V^T$  with the dimensions indicated by the rectangles.

$U$  is referred to as the **left-singular vector**,  
 $V$  is the **right-singular vector**,  
 $\Sigma$  are the **singular values** (increasing order)

# Singular Value Decomposition



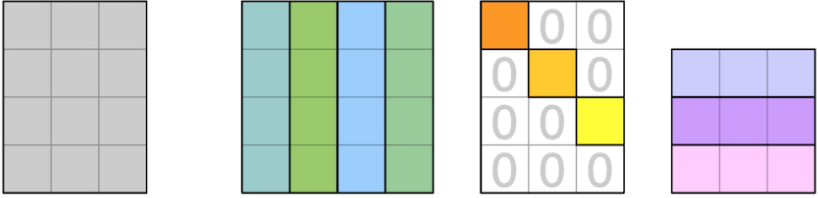
$$\begin{matrix} \mathbf{X} \\ n \times m \end{matrix} = \begin{matrix} \mathbf{U} \\ n \times n \end{matrix} \begin{matrix} \mathbf{\Sigma} \\ n \times m \end{matrix} \begin{matrix} \mathbf{V}^* \\ m \times m \end{matrix}$$

- Singular values matrix  $\Sigma$  has additional zero padding of rows or columns:

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & 0 & 0 & \dots & 0 \\ 0 & \ddots & 0 & \vdots & & \vdots \\ 0 & 0 & \sigma_n & 0 & \dots & 0 \end{bmatrix} \quad \text{when } n < m$$

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_m \\ 0 & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{bmatrix} \quad \text{when } m < n$$

# Singular Value Decomposition



$$\mathbf{A}_{n \times m} = \mathbf{U}_{n \times n} \mathbf{\Sigma}_{n \times m} \mathbf{V}^*_{m \times m}$$

	Ali	Beatrix	Chandra
Star Wars	5	4	1
Blade Runner	5	5	0
Amelie	0	0	5
Delicatessen	1	0	4

$$= \begin{bmatrix} \text{Sci-fi} & \text{French} \\ -0.6710 & 0.0236 & 0.4647 & -0.5774 \\ -0.7197 & 0.2054 & -0.4759 & 0.4619 \\ -0.0939 & -0.7705 & -0.5268 & -0.3464 \\ -0.1515 & -0.6030 & 0.5293 & -0.5774 \end{bmatrix}$$

$$\begin{bmatrix} 9.6438 & 0 & 0 \\ 0 & 6.3639 & 0 \\ 0 & 0 & 0.7056 \\ 0 & 0 & 0 \end{bmatrix}$$

	Sci-fi	French
Sci-fi	-0.7367	-0.6515
French	0.0852	0.1762
	0.6708	-0.7379

# Implications

- If we can decompose our matrix, then that can give us insights into our data.
- SVD is behind some of the many machine learning applications
  - recommender systems
  - word embeddings
  - image compressions
  - background removal

More on this later



# SVD Algorithm

- Finding the left and right singular vectors shares some similarities with PCA:
- Right-singular vectors:

$$X^T X = V D V^T$$

- Left-singular vectors:

$$X X^T = U D U^T$$

$$\begin{matrix} n \\ m \end{matrix} \boxed{X} = \begin{matrix} m \\ m \end{matrix} \boxed{U} \begin{matrix} n \\ m \end{matrix} \boxed{\Sigma} \begin{matrix} n \\ n \end{matrix} \boxed{V^T}$$

- $XX^T$  and  $X^T X$  are symmetrical
- SVD does not require that we normalized  $X$  to have zero mean

# SVD Algorithm

➤ Right-Singular:

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

eigendecomposition  
of  $X^T X$ , with  $\Sigma = \sqrt{D}$

➤ Left-Singular:


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

eigendecomposition  
of  $X X^T$  with  $\Sigma = \sqrt{D}$

# SVD Algorithm

- The right-singular vectors ( $V$ ) and left-singular vectors ( $U$ ) (which we know to be orthonormal) are connected through the singular value matrix:

$$AV = U\Sigma$$

$$Av_i = \sigma_i u_i \quad i = 1, \dots, r$$


$\min(m, n)$

## Example 4.13

Compute the singular value decomposition for matrix A.

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





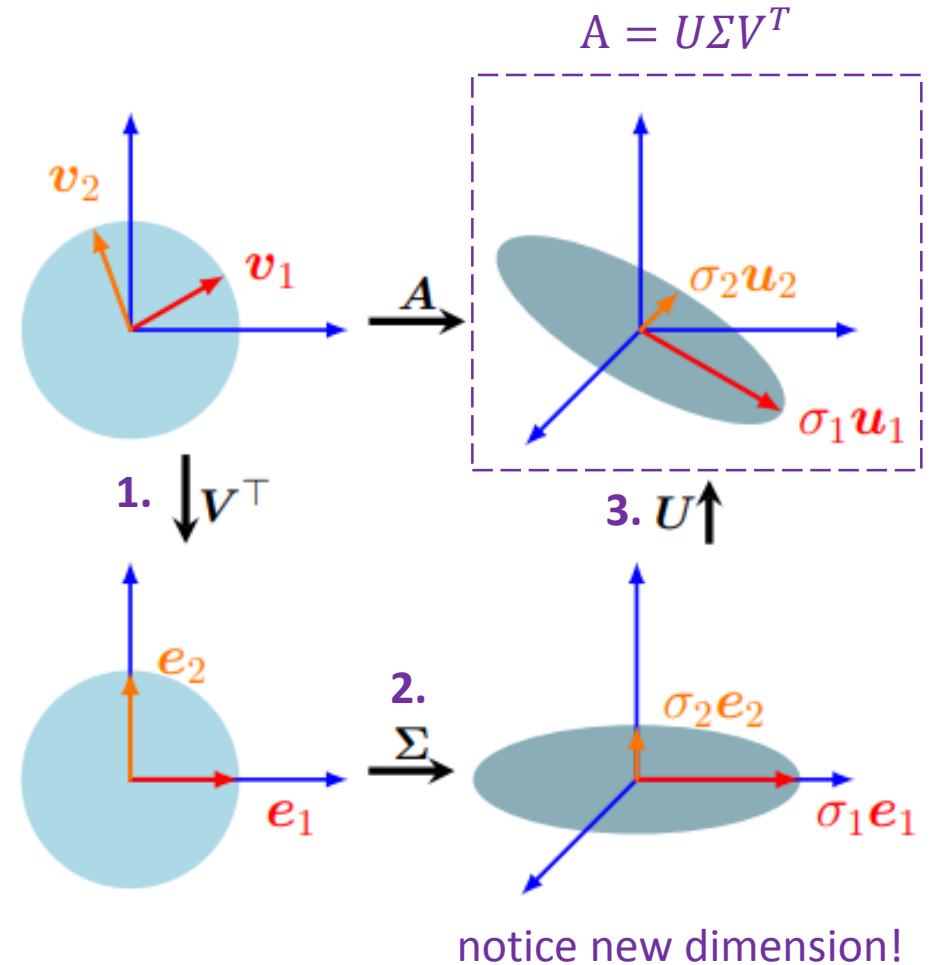
# Geometric Interpretation of SVD

- A rectangular matrix (n x m) can be factored into:

$$A = U\Sigma V^T$$

- These can be seen as a sequence of transformations:

1. rotation by right-singular  $V$
2. scaling by singular values  $\Sigma$
3. rotation by left-singular again  $U$



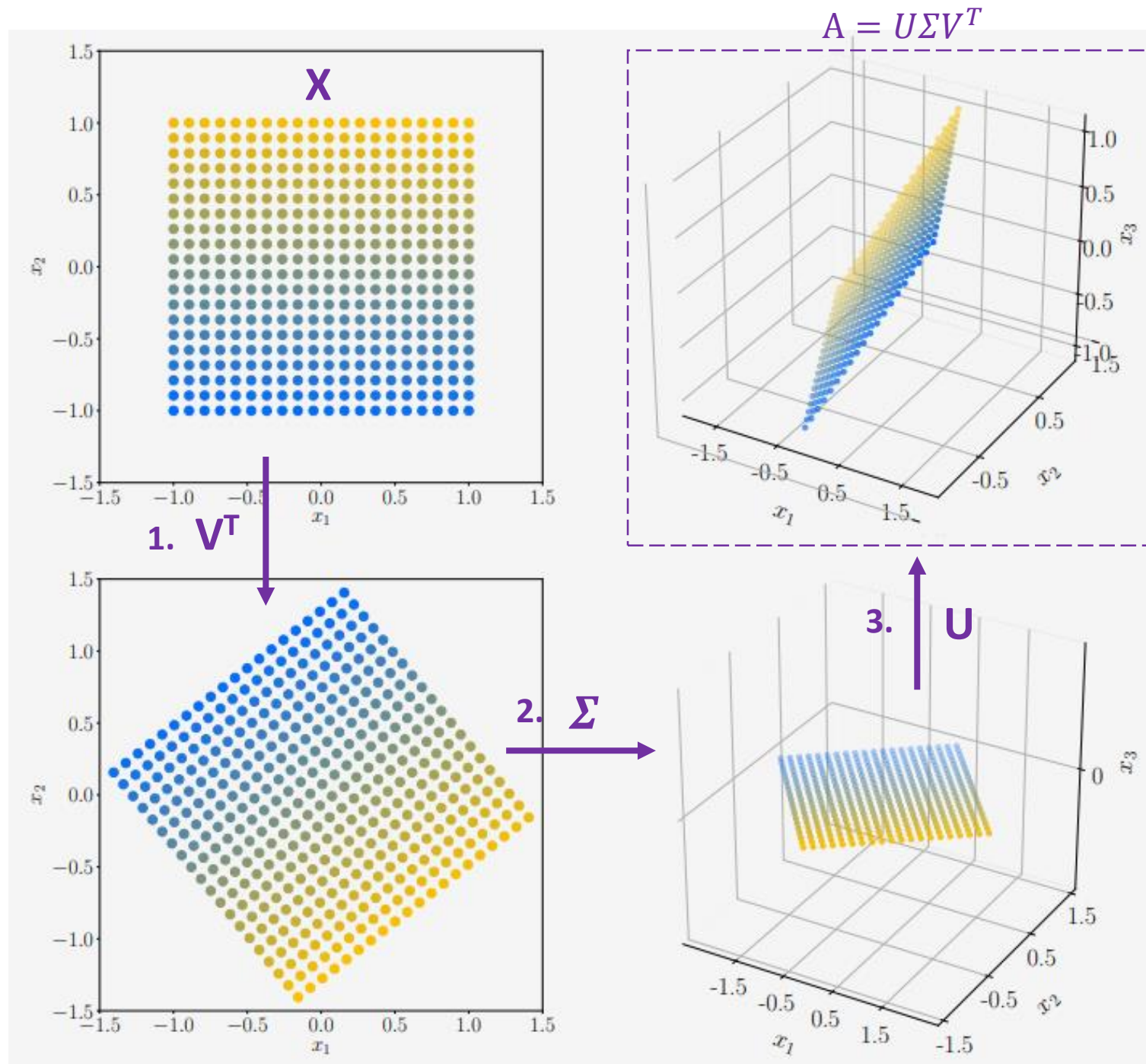
# Example

Given: A set of data points  $X$  and transformation  $A$ .

$$\begin{aligned} A &= \begin{bmatrix} 1 & -0.8 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} = U \Sigma V^T \\ &= \begin{bmatrix} -0.79 & 0 & -0.62 \\ 0.38 & -0.78 & -0.49 \\ -0.48 & -0.62 & 0.62 \end{bmatrix} \begin{bmatrix} 1.62 & 0 \\ 0 & 1.0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -0.78 & 0.62 \\ -0.62 & -0.78 \end{bmatrix} \end{aligned}$$

$X \rightarrow$  set of vectors

1.  $V^T \rightarrow$  rotates data  $X$
2.  $\Sigma \rightarrow$  singular matrix maps onto  $\mathbb{R}^3$  (3<sup>rd</sup> dimension is 0, stretched in a plane by singular values)
3.  $U \rightarrow$  rotation within  $\mathbb{R}^3$





# Similarities to Eigendecomposition -1

## ➤ Eigenvalue Decomposition vs Singular Value Decomposition:

- SVD exists for any matrix (m x n) whether square or rectangular
- SVD left and right singular vectors can be made orthonormal
- Both are a composition of three linear mappings:
  1. Change of basis in the domain
  2. Independent scaling of each new basis vector from domain to codomain
  3. Change of basis in codomain
- SVD domain and codomain can be vector spaces of different dimensions.

Eigendecomposition

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

Singular Value Decomposition

$$X = U\Sigma V^T$$

# Similarities to Eigendecomposition -2

- SVD singular values are real and non-negative
- SVD and eigendecomposition are closely related through their projections:
  - The left-singular vectors of  $A$  are eigenvectors of  $AA^T$
  - The right-singular vectors of  $A$  are eigenvectors of  $A^TA$
  - The nonzero singular values of  $A$  are the square roots of nonzero eigenvalues of  $AA^T$  and  $A^TA$
- **For symmetric square matrices ( $n \times n$ ) eigendecomposition and SVD are the same when features are normalized**

Eigendecomposition

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

Singular Value  
Decomposition

$$X = U\Sigma V^T$$

$$\longrightarrow P = U = V$$

# Relationship between PCA and SVD

- PCA and SVD are closely related:

$$\begin{aligned} \text{Cov}(A) &= \frac{X^T X}{n-1} \\ &= \frac{(U \Sigma V^T)^T (U \Sigma V^T)}{n-1} \\ &= \frac{V \Sigma U^T U \Sigma V^T}{n-1} \\ &= V \frac{\Sigma^2}{n-1} V^T \end{aligned}$$

$$\begin{matrix} n \\ m \end{matrix} \begin{matrix} X \end{matrix} = \begin{matrix} m \\ m \end{matrix} \begin{matrix} U \end{matrix} \begin{matrix} m \\ n \end{matrix} \begin{matrix} \Sigma \end{matrix} \begin{matrix} n \\ n \end{matrix} \begin{matrix} V^T \end{matrix}$$

SVD columns of  $V$  are principal direction in PCA

- The result is the same form as eigendecomposition of  $A$  and hence:

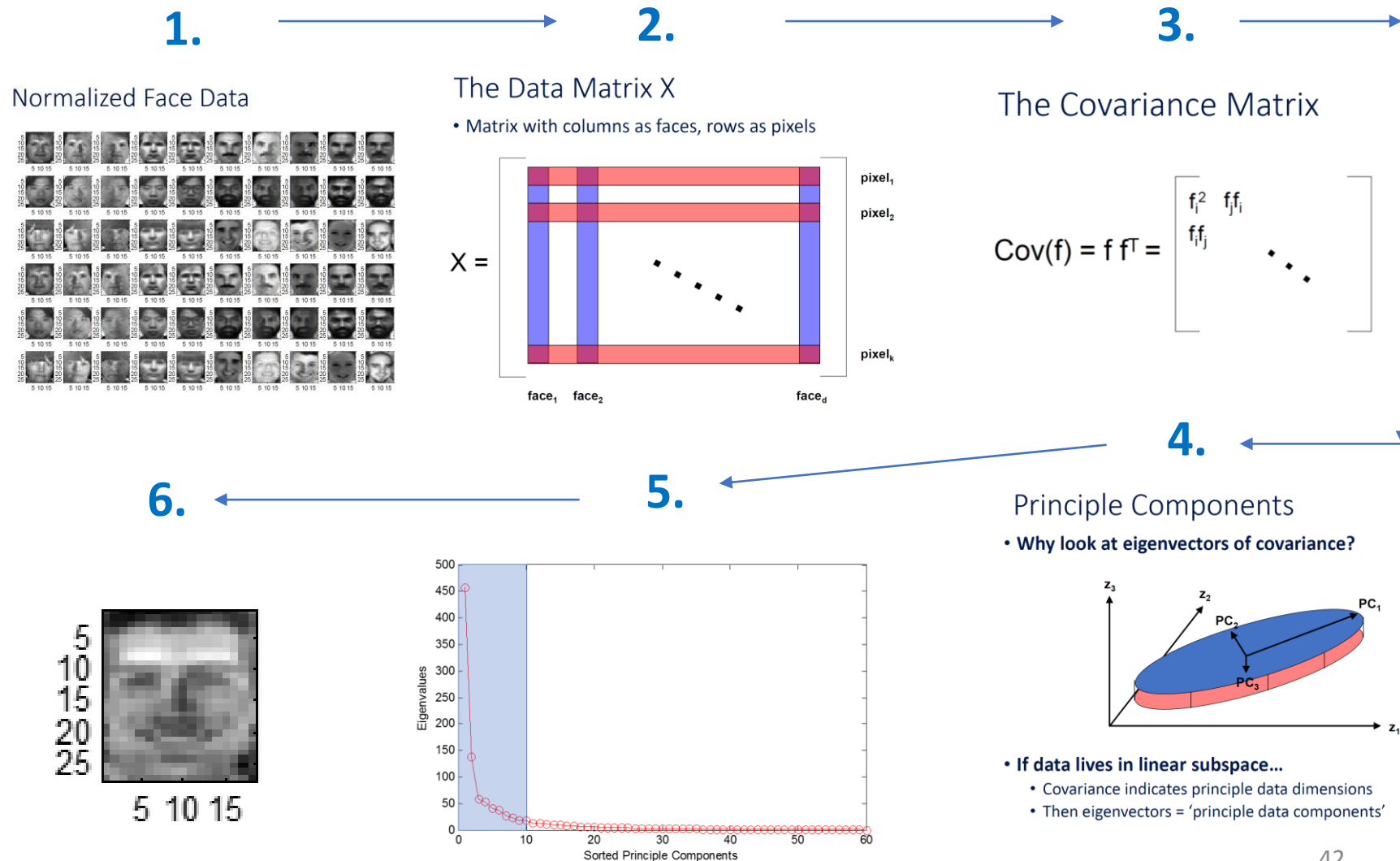
$$\begin{matrix} \nearrow \\ \text{eigenvalues} \end{matrix} \begin{matrix} D \end{matrix} = \frac{\begin{matrix} \boxed{\Sigma^2} \\ \nwarrow \\ \text{singular values} \end{matrix}}{n-1}$$

# Applications of Matrix Decompositions

**Dimensionality Reduction**  
**Data Interpretation**

# Recap: Eigenfaces

➤ Last time we saw how PCA could be used to obtain a compressed version of face images.



# Image Compression

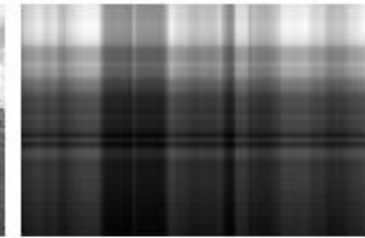
- Analogous to decomposing face we can also decompose a single image for compression.

$$A = U\Sigma V^T \in \mathbb{R}^{m \times n}$$

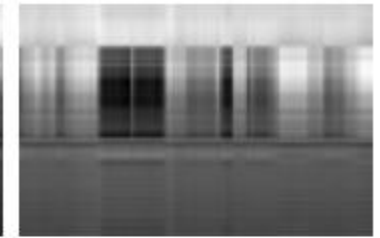
$$A = \sum_{i=1}^r \sigma_i u_i v_i^T = \sum_{i=1}^r \sigma_i A_i$$



(a) Original image  $A$ .



(b) Rank-1 approximation  $\hat{A}(1)$ .



(c) Rank-2 approximation  $\hat{A}(2)$ .



(d) Rank-3 approximation  $\hat{A}(3)$ .



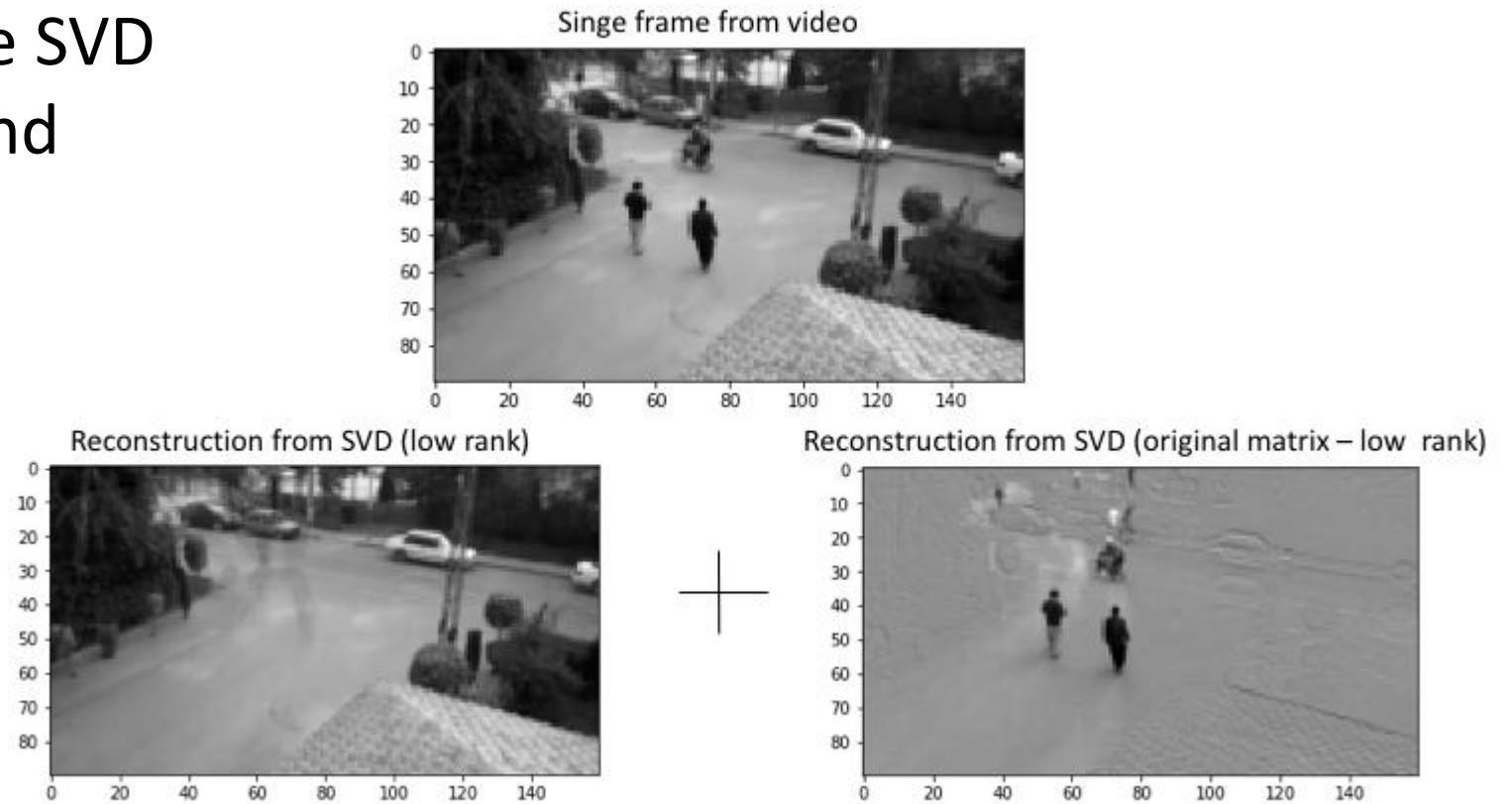
(e) Rank-4 approximation  $\hat{A}(4)$ .



(f) Rank-5 approximation  $\hat{A}(5)$ .

# Application 1 – Background Removal

- Given a video we can use SVD to remove the background



# Example Google Colab Code



# Application 2 – Recommender Systems

➤ SVD can also be used to find structure in data for making recommendations.

➤ SVD is strongly related to recommender systems applications:

- Movie recommendations
- Product recommendations
- Restaurant recommendations
- Website recommendations
- ...

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Star Wars	5	4	1
Blade Runner	5	5	0
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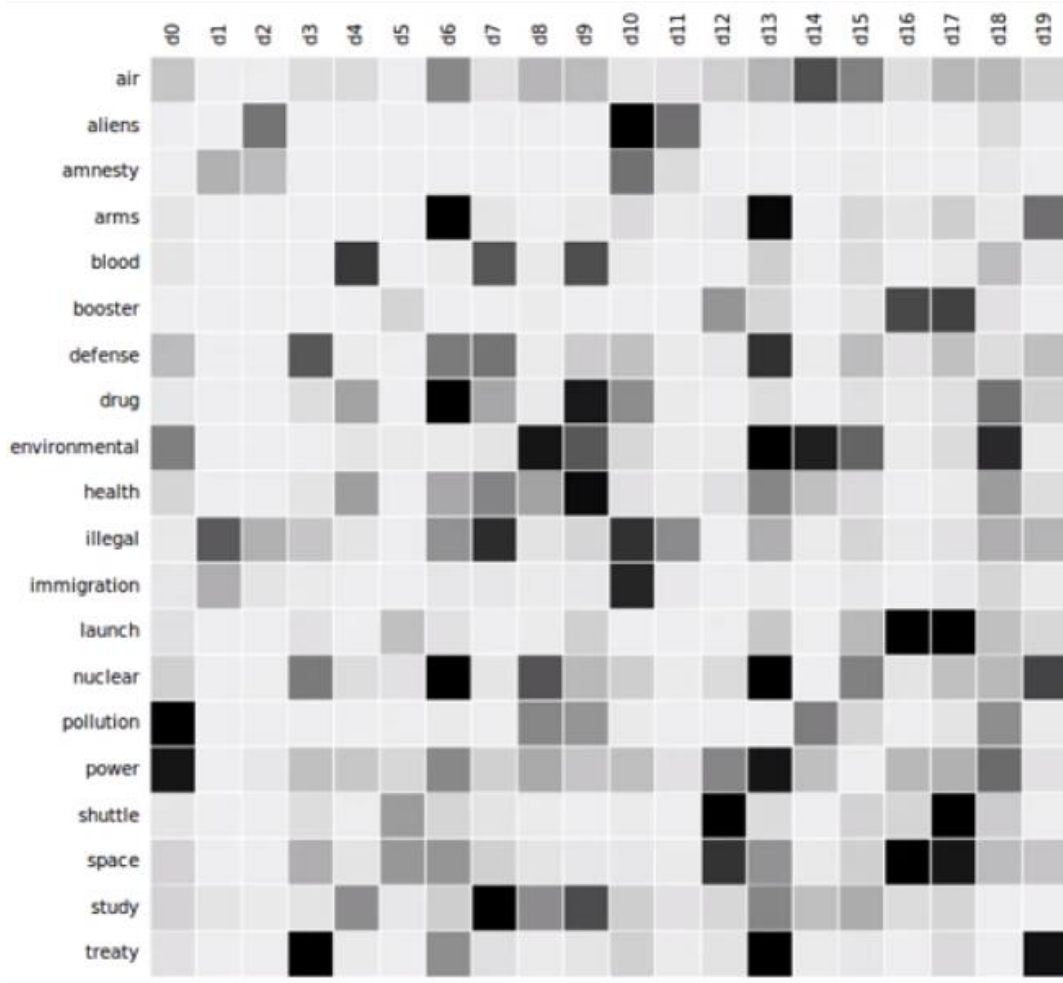
$$= \begin{bmatrix} -0.6710 & 0.0236 & 0.4647 & -0.5774 \\ -0.7197 & 0.2054 & -0.4759 & 0.4619 \\ -0.0939 & -0.7705 & -0.5268 & -0.3464 \\ -0.1515 & -0.6030 & 0.5293 & -0.5774 \end{bmatrix}$$

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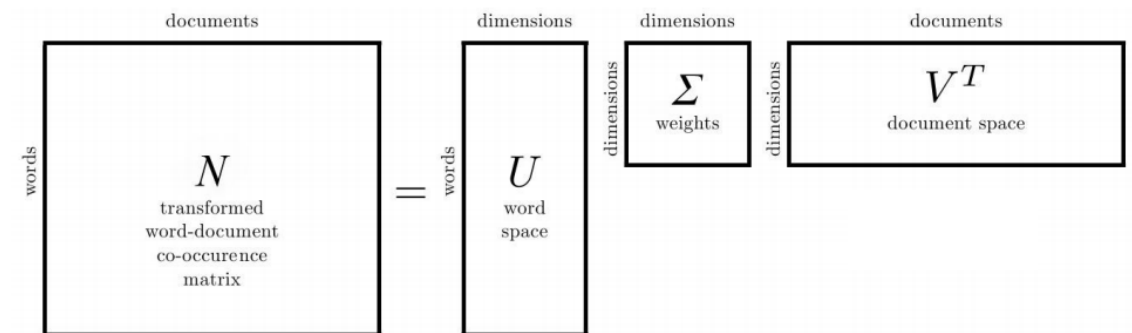
# Example Google Colab Code

# Application 3 – Text Embeddings



Source: Wikipedia

- Word relationships from documents
  - Latent semantic representation



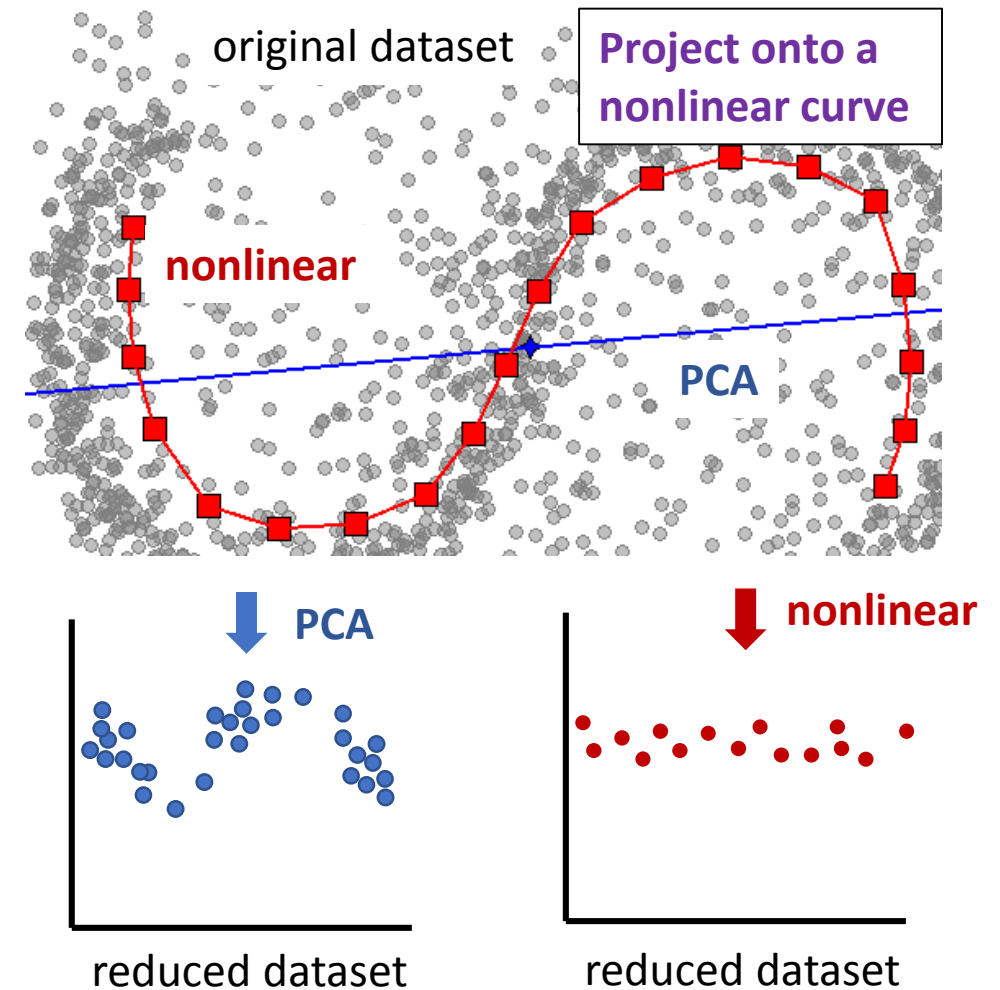
# Example Google Colab Code

# Summary

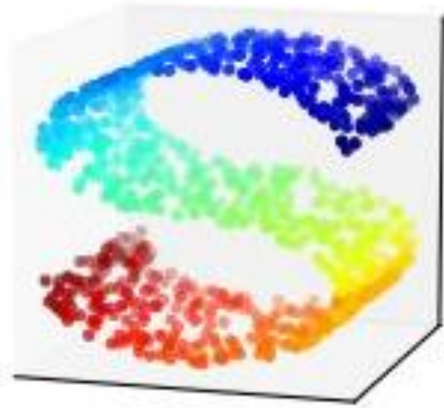
- Eigendecomposition and Singular Value Decomposition offer ways to factor matrices, much like we can factor numbers into primary numbers.
- This can lead to dimensionality reduction, data insights and algorithm speed ups.
- Eigendecomposition is limited to square matrices, so we use **SVD which is guaranteed to work in all circumstances.**
- **(limitation) Both apply linear transformations/mappings**

# Nonlinear Dimensionality Reduction

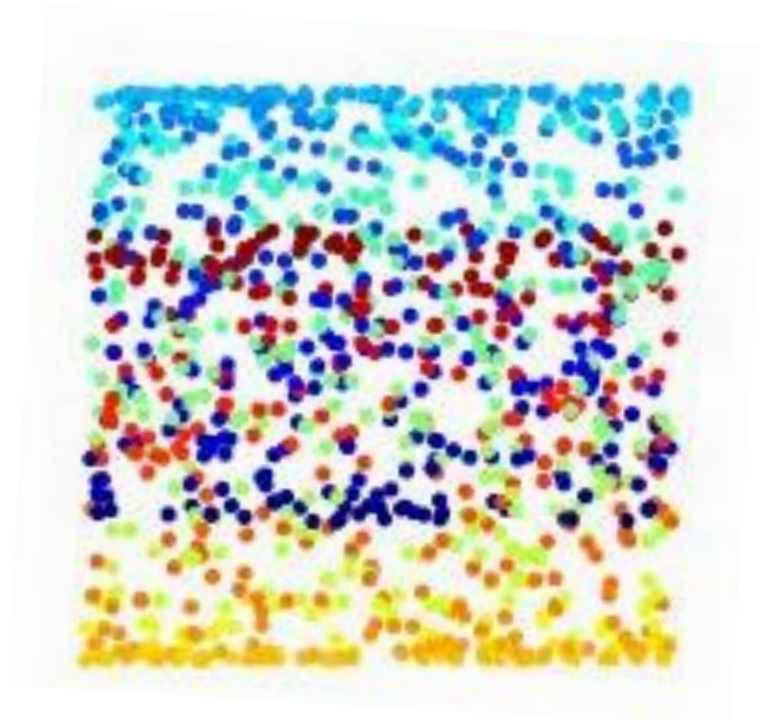
- Data can have nonlinear relationships for which our decomposition techniques would be ineffective.
- Nonlinear Data Visualization/Reduction
  - t-SNE
  - Isomap
  - LLE
  - Kernel PCA
  - Deep Autoencoders  
(type of neural network)



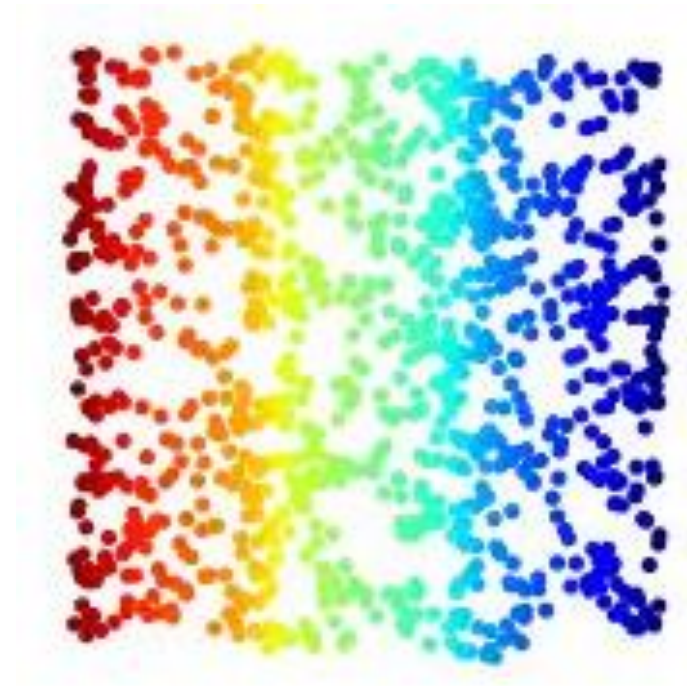
# Example: Nonlinear Projections



Nonlinear Data



PCA Projection



Isomap Projection

# Vector Calculus

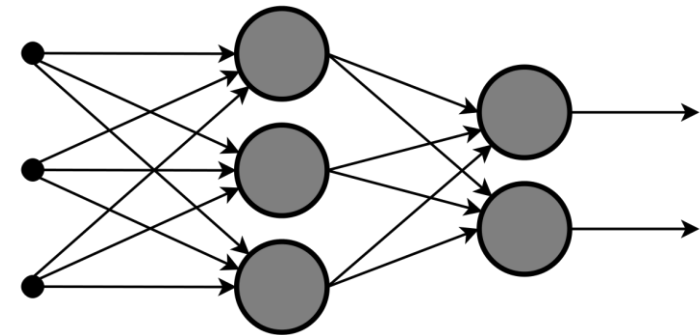
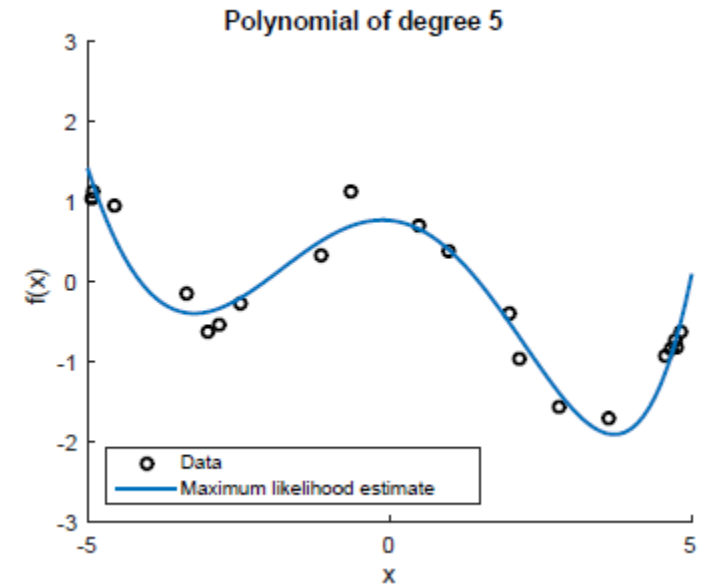
**Readings:**

- **MML Chapter 5.1-4**



# Why Vector Calculus?

- Vector calculus is used extensively in optimization
  - We will see it the next couple lectures when we discuss model-based learning using **linear regression** and **neural network models**
- Most of the python frameworks such as Tensorflow, PyTorch, etc. handle these calculations using numerical methods



# Types of Differentiation

1. Scalar differentiation:  $f : \mathbb{R} \rightarrow \mathbb{R}$

$y \in \mathbb{R}$  w.r.t.  $x \in \mathbb{R}$

2. Multivariate case:  $f : \mathbb{R}^N \rightarrow \mathbb{R}$

$y \in \mathbb{R}$  w.r.t. vector  $x \in \mathbb{R}^N$

3. Vector fields:  $f : \mathbb{R}^N \rightarrow \mathbb{R}^M$

vector  $y \in \mathbb{R}^M$  w.r.t. vector  $x \in \mathbb{R}^N$

4. General derivatives:  $f : \mathbb{R}^{M \times N} \rightarrow \mathbb{R}^{P \times Q}$

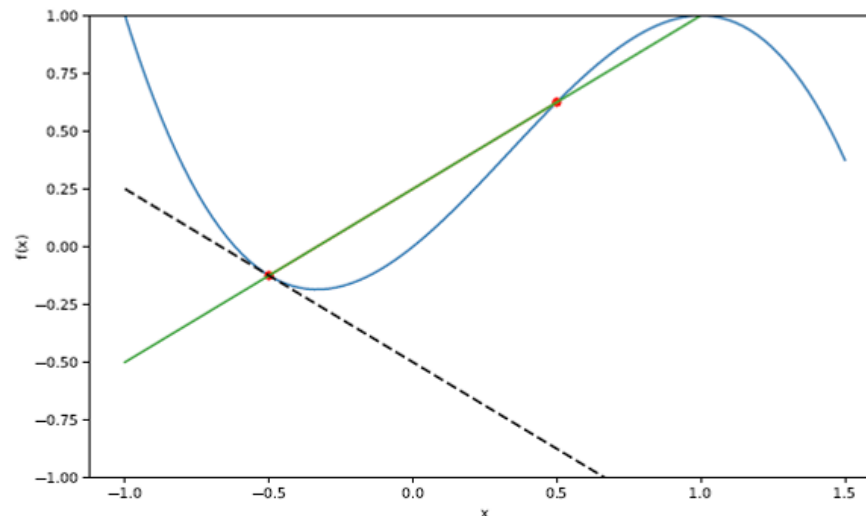
matrix  $y \in \mathbb{R}^{P \times Q}$  w.r.t. matrix  $X \in \mathbb{R}^{M \times N}$

# 1. Scalar Differentiation

- Derivative defined as the limit of the difference quotient:

$$f'(x) = \frac{df}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

- Slope of a secant line through  $f(x)$  and  $f(x+h)$



# Some Examples

$$f(x) = x^n$$

$$f'(x) = nx^{n-1}$$

$$f(x) = \sin(x)$$

$$f'(x) = \cos(x)$$

$$f(x) = \tanh(x)$$

$$f'(x) = 1 - \tanh^2(x)$$

$$f(x) = \exp(x)$$

$$f'(x) = \exp(x)$$

$$f(x) = \log(x)$$

$$f'(x) = \frac{1}{x}$$

# Rules

- ▶ Sum Rule

$$(f(x) + g(x))' = f'(x) + g'(x) = \frac{df(x)}{dx} + \frac{dg(x)}{dx}$$

- ▶ Product Rule

$$(f(x)g(x))' = f'(x)g(x) + f(x)g'(x) = \frac{df(x)}{dx}g(x) + f(x)\frac{dg(x)}{dx}$$

- ▶ Chain Rule

$$(g \circ f)'(x) = (g(f(x)))' = g'(f(x))f'(x) = \frac{dg(f(x))}{df} \frac{df(x)}{dx}$$

- ▶ Quotient Rule

$$\left(\frac{f(x)}{g(x)}\right)' = \frac{f(x)'g(x) - f(x)g(x)'}{(g(x))^2} = \frac{\frac{df}{dx}g(x) - f(x)\frac{dg}{dx}}{(g(x))^2}$$

# Example: Scalar Chain Rule

$$(g \circ f)'(x) = (g(f(x)))' = g'(f(x))f'(x) = \frac{dg}{df} \frac{df}{dx}$$

$$g(z) = 6z + 3$$

$$z = f(x) = -2x + 5$$

$$\begin{aligned}(g \circ f)'(x) &= \underbrace{(6)}_{dg/df} \underbrace{(-2)}_{df/dx} \\ &= -12\end{aligned}$$

## 2. Multivariate Differentiation $f: \mathbb{R}^N$ to $\mathbb{R}$

$$y = f(\mathbf{x}),$$

➤ Partial derivative (change one coordinate at a time)

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^N$$

$$\frac{\partial f}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_N) - f(\mathbf{x})}{h}$$

➤ The gradient collects all partial derivatives:

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{1 \times N} \quad \text{results in a row vector}$$

# Example: Multivariate Differentiation

➤ Given:

$$f : \mathbb{R}^2 \rightarrow \mathbb{R}$$

$$f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$$

➤ Partial derivative

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2x_1 x_2 + x_2^3$$

$$\frac{\partial f(x_1, x_2)}{\partial x_2} = x_1^2 + 3x_1 x_2^2$$

➤ Gradient

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f(x_1, x_2)}{\partial x_1} & \frac{\partial f(x_1, x_2)}{\partial x_2} \end{bmatrix} \in \mathbb{R}^{1 \times 2}$$

$$= \begin{bmatrix} 2x_1 x_2 + x_2^3 & x_1^2 + 3x_1 x_2^2 \end{bmatrix}$$



### 3. Vector Field Differentiation $f: \mathbb{R}^N \rightarrow \mathbb{R}^M$

$$\mathbf{y} = \mathbf{f}(\mathbf{x}) \in \mathbb{R}^M, \quad \mathbf{x} \in \mathbb{R}^N$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_M(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} f_1(x_1, \dots, x_N) \\ \vdots \\ f_M(x_1, \dots, x_N) \end{bmatrix}$$

➤ Jacobian matrix (collection of all partial derivatives)

$$\begin{bmatrix} \frac{dy_1}{dx} \\ \vdots \\ \frac{dy_M}{dx} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \dots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{M \times N}$$

# Example: Vector Field Differentiation

➤ Given:  $f(x) = Ax$ ,  $f(x) \in \mathbb{R}^M$ ,  $A \in \mathbb{R}^{M \times N}$ ,  $x \in \mathbb{R}^N$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(x) \\ \vdots \\ f_M(x) \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + \cdots + A_{1N}x_N \\ \vdots \\ A_{M1}x_1 + A_{M2}x_2 + \cdots + A_{MN}x_N \end{bmatrix}$$

➤ Compute the Jacobian

$$f_i(x) = \sum_{j=1}^N A_{ij}x_j$$
$$\frac{\partial f_i}{\partial x_j} = A_{ij}$$
$$\frac{df}{dx} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MN} \end{bmatrix} = A \in \mathbb{R}^{M \times N}$$

# Dimensionality

- In general: A function  $f: \mathbb{R}^N \rightarrow \mathbb{R}^M$  has a result that is an  $M \times N$  matrix with:

$$\frac{df}{dx} \in \mathbb{R}^{M \times N}, \quad df[m, n] = \frac{\partial f_m}{\partial x_n}$$

Gradient dimension: #target dimensions x #input dimensions

# Example: Chain Rule

➤ Given  $f: \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $x: \mathbb{R} \rightarrow \mathbb{R}^2$

$$f(x) = f(x_1, x_2) = x_1^2 + 2x_2,$$

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \sin(t) \\ \cos(t) \end{bmatrix}$$

➤ What are the dimensions of  $df/dx$  and  $dx/dt$ ?

$1 \times 2$  and  $2 \times 1$

➤ Compute  $df/dt$  using the chain rule:

$$\begin{aligned} \frac{df}{dt} &= \frac{df}{dx} \frac{dx}{dt} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix} = \begin{bmatrix} 2 \sin t & 2 \end{bmatrix} \begin{bmatrix} \cos t \\ -\sin t \end{bmatrix} \\ &= 2 \sin t \cos t - 2 \sin t = 2 \sin t (\cos t - 1) \end{aligned}$$

# 4. Derivatives with Respect to Matrices

- Recall: A function  $f: \mathbb{R}^N \rightarrow \mathbb{R}^M$  has a Jacobian that is an  $M \times N$  matrix with:

$$\frac{df}{dx} \in \mathbb{R}^{M \times N}, \quad df[m, n] = \frac{\partial f_m}{\partial x_n}$$

Gradient dimension: #target dimensions x #input dimensions

- This generalizes to when the inputs (N) or targets (M) are **matrices**.

- Function  $f: \mathbb{R}^{M \times N} \rightarrow \mathbb{R}^{P \times Q}$  has a Jacobian that is a  $(P \times Q) \times (M \times N)$  **tensor**:

$$\frac{df}{dX} \in \mathbb{R}^{(P \times Q) \times (M \times N)}, \quad df[p, q, m, n] = \frac{\partial f_{pq}}{\partial X_{mn}}$$

# More Examples:

# Example:

➤ Given:  $f(x) = Ax$ ,  $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ ,  $x = [x_1 \ x_2]^T$

➤ Find  $df(x)/dx$

# Example:

➤ Given:  $f(x) = x^T A x$ ,  $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ ,  $x = [x_1 \ x_2]^T$

➤ Find  $df(x)/dx$



# Example: PCA Derivation

- Requires some familiarity with vector calculus for matrix differentiation
- There are three perspectives:
  1. Maximum Variance Perspective
  2. Projection Perspective
  3. Latent Variable Perspective
- Lead to the same result using different derivations.
- **Suggested derivation:** [Deep Learning Textbook \(pgs 45 – 50\)](#) by Ian Goodfellow, Yoshua Bengio and Aaron Courville.

# Next Time

- Week 8 Support Session
  - Project 3 Support
- Reading Assignment
- Lecture – Linear Regression
  - Data, Models and Learning
  - Empirical Risk Minimization
  - Maximum Likelihood
  - Probabilistic Modelling and Inference