

# CSC 311: Introduction to Machine Learning

## Lecture 10 - PCA, Matrix Completion, Autoencoders

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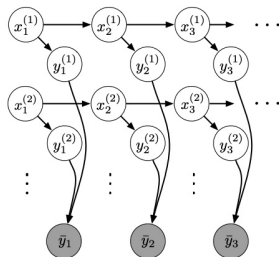
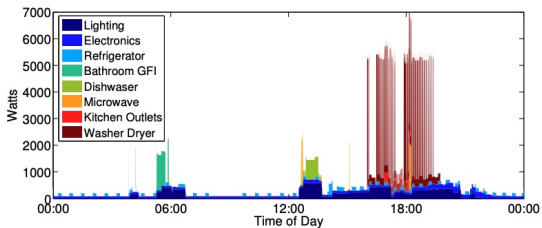
University of Toronto, Fall 2022

# Today

- So far in this course: supervised learning
- Today we start unsupervised learning
  - ▶ No labels, so the purpose is to find patterns in data
  - ▶ Need to specify what kind of patterns to look for
- **This week:** dimensionality reduction
  - ▶ Linear dimensionality reduction (Principal Component Analysis)
    - ▶ Matrix completion (needed for the project) is closely related to PCA.
  - ▶ Nonlinear dimensionality reduction (autoencoders)
- **Week 11:** clustering

# Motivating Examples

## Energy disaggregation



Kolter and Johnson, "REDD: A public data set for energy disaggregation research"

# Motivating Examples

## Modeling the change in scientific topics over time

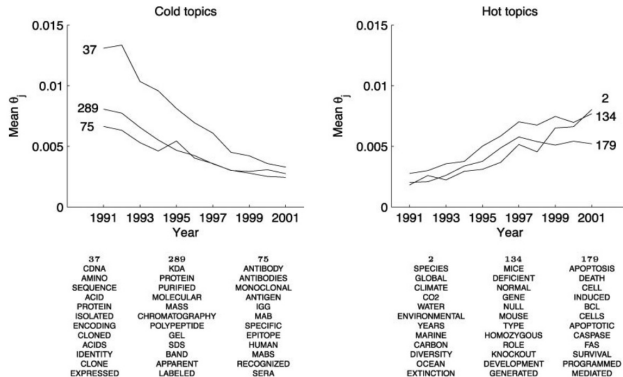
217 INSECT MYB PHEROMONE LENS LARVAE	274 SPECIES PHYLOGENETIC EVOLUTION EVOLUTIONARY SEQUENCES	126 GENE VECTOR VECTORS EXPRESSION TRANSFER	63 STRUCTURE ANGSTROM CRYSTAL RESIDUES STRUCTURES	200 FOLDING NATIVE PROTEIN STATE ENERGY	209 NUCLEAR NUCLEUS LOCALIZATION CYTOPLASM EXPORT
42 NEURAL DEVELOPMENT DORSAL EMBRYOS VENTRAL	2 SPECIES GLOBAL CLIMATE CO2 WATER	280 SPECIES SELECTION EVOLUTION GENETIC POPULATIONS	15 CHROMOSOME REGION CHROMOSOMES KB MAP	64 CELLS CELL ANTIGEN LYMPHOCYTES CD4	102 TUMOR CANCER TUMORS HUMAN CELLS

A generalized<sup>1</sup> fundamental<sup>1,48</sup> theorem<sup>287</sup> of natural<sup>250</sup> selection<sup>250</sup> is derived<sup>251</sup> for populations<sup>250</sup> incorporating<sup>1,49</sup> both genetic<sup>250</sup> and cultural<sup>250</sup> transmission<sup>251</sup>. The phenotype<sup>2</sup> is determined<sup>2</sup> by an arbitrary<sup>2</sup> number<sup>27</sup> of multiallelic<sup>2</sup> loci with two<sup>77</sup>-factor<sup>69</sup> epistasis<sup>240</sup> and an arbitrary<sup>1,49</sup> linkage<sup>2</sup> map<sup>2</sup>, as well as by cultural<sup>150</sup> transmission<sup>27</sup> from the parents<sup>250</sup>. Generations<sup>250</sup> are discrete<sup>69</sup> but partially<sup>27</sup> overlapping<sup>25</sup>, and mating<sup>250</sup> may be nonrandom<sup>250</sup> at either the genotypic<sup>250</sup> or the phenotypic<sup>250</sup> level<sup>250</sup> (or both). I show<sup>27</sup> that cultural<sup>150</sup> transmission<sup>27</sup> has several<sup>27</sup> important<sup>27</sup> implications<sup>27</sup> for the evolution<sup>250</sup> of population<sup>150</sup> fitness<sup>250</sup>, most notably<sup>210</sup> that there is a time<sup>2</sup> lag<sup>2</sup> in the response<sup>212</sup> to selection<sup>250</sup> such that the future<sup>27</sup> evolution<sup>250</sup> depends<sup>107</sup> on the past selection<sup>250</sup> history<sup>250</sup> of the population<sup>250</sup>.

Griffiths and Steyvers, "Finding scientific topics"

# Motivating Examples

Modeling the change in scientific topics over time

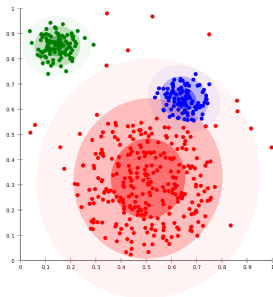


Griffiths and Steyvers, "Finding scientific topics"

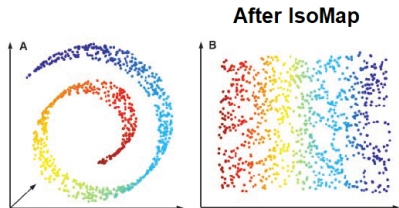
# Motivating Examples

The models for those tasks are fairly complicated. In this course, we'll focus on two simpler instances of unsupervised learning:

## Clustering



## Dimensionality Reduction



# Linear Dimensionality Reduction

- We'll start with a simpler form of dimensionality reduction: **linear dimensionality reduction**
- **Example:** suppose you're a psychologist interested in modeling the variation in human personality
  - ▶ You've asked lots of participants to take a survey with lots of personality questions.
  - ▶ By figuring out which questions are highly correlated with each other, you can uncover the main factors describing human personality.
- A linear dimensionality reduction model called **factor analysis** found five key personality traits called the Big Five:
  - ▶ extraversion, agreeableness, openness to experience, conscientiousness, neuroticism
- In this lecture, we'll consider a different but closely related model called **Principal Component Analysis (PCA)**.

# PCA: Overview

- Principal Component Analysis (PCA) is our first unsupervised learning algorithm, and an example of linear dimensionality reduction.
- **Dimensionality reduction:** map data to a lower dimensional space
  - ▶ Save computation/memory
  - ▶ Reduce overfitting, achieve better generalization
  - ▶ Visualize in 2 dimensions
- Since PCA is a linear model, this mapping will be a **projection**.

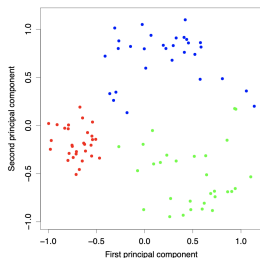
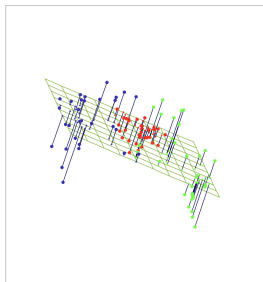
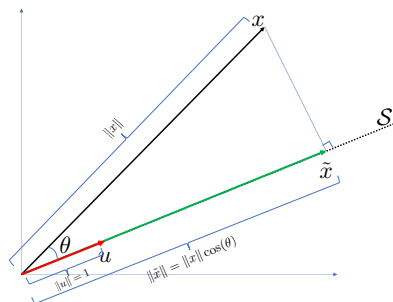


Image credit: Elements of Statistical Learning



# Euclidean projection

## Projection onto a 1-D subspace



- Subspace  $\mathcal{S}$  is the line along the unit vector  $\mathbf{u}$ 
  - ▶  $\{\mathbf{u}\}$  is a **basis** for  $\mathcal{S}$ : any point in  $\mathcal{S}$  can be written as  $z\mathbf{u}$  for some  $z$ .

- Projection of  $\mathbf{x}$  on  $\mathcal{S}$  is denoted by  $\text{Proj}_{\mathcal{S}}(\mathbf{x})$
- Recall:  $\mathbf{x}^{\top} \mathbf{u} = \|\mathbf{x}\| \|\mathbf{u}\| \cos(\theta) = \|\mathbf{x}\| \cos(\theta)$
- $\text{Proj}_{\mathcal{S}}(\mathbf{x}) = \underbrace{\mathbf{x}^{\top} \mathbf{u}}_{\text{length of proj}} \cdot \underbrace{\mathbf{u}}_{\text{direction of proj}} = \|\tilde{\mathbf{x}}\| \mathbf{u}$

# General subspaces

- How to project onto a  $K$ -dimensional subspace?
  - ▶ **Idea:** choose an orthonormal basis  $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_K\}$  for  $\mathcal{S}$  (i.e. all unit vectors and orthogonal to each other)
  - ▶ Project onto each unit vector individually (as in previous slide), and sum together the projections.
- Mathematically, the projection is given as:

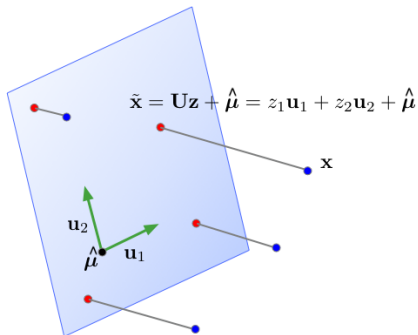
$$\text{Proj}_{\mathcal{S}}(\mathbf{x}) = \sum_{i=1}^K z_i \mathbf{u}_i \quad \text{where} \quad z_i = \mathbf{x}^\top \mathbf{u}_i.$$

- In vector form:

$$\text{Proj}_{\mathcal{S}}(\mathbf{x}) = \mathbf{U}\mathbf{z} \quad \text{where} \quad \mathbf{z} = \mathbf{U}^\top \mathbf{x}$$

# Projection onto a Subspace

- So far, we assumed the subspace passes through  $\mathbf{0}$ .
- In mathematical terminology, the “subspaces” we want to project onto are really **affine spaces**, and can have an arbitrary origin  $\hat{\boldsymbol{\mu}}$ .

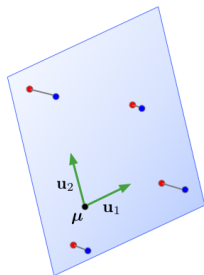


$$\mathbf{z} = \mathbf{U}^T(\mathbf{x} - \hat{\boldsymbol{\mu}})$$

- In machine learning,  $\tilde{\mathbf{x}}$  is also called the **reconstruction** of  $\mathbf{x}$ .
- $\mathbf{z}$  is its **representation**, or **code**.

# Projection onto a Subspace

- If we have a  $K$ -dimensional subspace in a  $D$ -dimensional input space, then  $\mathbf{x} \in \mathbb{R}^D$  and  $\mathbf{z} \in \mathbb{R}^K$ .
- If the data points  $\mathbf{x}$  all lie close to their reconstructions, then we can approximate distances, etc. in terms of these same operations on the code vectors  $\mathbf{z}$ .
- If  $K \ll D$ , then it's much cheaper to work with  $\mathbf{z}$  than  $\mathbf{x}$ .
- A mapping to a space that's easier to manipulate or visualize is called a **representation**, and learning such a mapping is **representation learning**.
- Mapping data to a low-dimensional space is called **dimensionality reduction**.



# Learning a Subspace

- How to choose a good subspace  $\mathcal{S}$ ?
  - ▶ Origin  $\hat{\boldsymbol{\mu}}$  is the empirical mean of the data
  - ▶ Need to choose a  $D \times K$  matrix  $\mathbf{U}$  with orthonormal columns.
- Two criteria:
  - ▶ Minimize the **reconstruction error**:

$$\min_{\mathbf{U}} \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}^{(i)} - \tilde{\mathbf{x}}^{(i)}\|^2$$

- ▶ Maximize the **variance of reconstructions**: Find a subspace where data has the most variability.

$$\max_{\mathbf{U}} \frac{1}{N} \sum_i \|\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}\|^2$$

- ▶ Note: The data and its reconstruction have the same means (exercise)!

# Learning a Subspace

- These two criteria are equivalent! I.e., we'll show

$$\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}^{(i)} - \tilde{\mathbf{x}}^{(i)}\|^2 = \text{const} - \frac{1}{N} \sum_i \|\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}\|^2$$

- Recall  $\tilde{\mathbf{x}}^{(i)} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{z}^{(i)}$  and  $\mathbf{z}^{(i)} = \mathbf{U}^\top(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})$ .

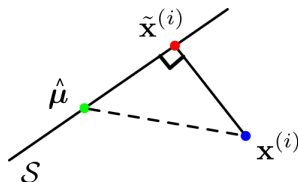
- **Observation 1:** Because the columns of  $\mathbf{U}$  are orthogonal,  $\mathbf{U}^\top\mathbf{U} = \mathbf{I}$ , so

$$\|\tilde{\mathbf{x}} - \hat{\boldsymbol{\mu}}\|^2 = \|\mathbf{U}\mathbf{z}\|^2 = \mathbf{z}^\top \mathbf{U}^\top \mathbf{U} \mathbf{z} = \mathbf{z}^\top \mathbf{z} = \|\mathbf{z}\|^2.$$

$\implies$  norm of centered reconstruction is equal to norm of representation.  
(If you draw it, this is obvious).

# Pythagorean Theorem

- Observation 1:  $\|\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}\|^2 = \|\mathbf{z}^{(i)}\|^2$ 
  - ▶ Variance of reconstructions is equal to variance of code vectors:  
 $\frac{1}{N} \sum_i \|\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}\|^2 = \frac{1}{N} \sum_i \|\mathbf{z}^{(i)}\|^2$  (exercise  $\frac{1}{N} \sum_i \mathbf{z}^{(i)} = 0$ )
- **Observation 2:** orthogonality of  $\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}$  and  $\tilde{\mathbf{x}}^{(i)} - \mathbf{x}^{(i)}$   
(Two vectors  $\mathbf{a}, \mathbf{b}$  are orthogonal  $\iff \mathbf{a}^\top \mathbf{b} = 0$ )
- Recall  $\tilde{\mathbf{x}}^{(i)} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{U}^\top (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})$ .



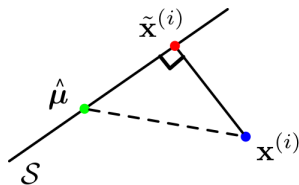
$$\begin{aligned} & (\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}})^\top (\tilde{\mathbf{x}}^{(i)} - \mathbf{x}^{(i)}) \\ &= (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top \mathbf{U}\mathbf{U}^\top (\hat{\boldsymbol{\mu}} - \mathbf{x}^{(i)} + \mathbf{U}\mathbf{U}^\top (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})) \\ &= (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top \mathbf{U}\mathbf{U}^\top (\hat{\boldsymbol{\mu}} - \mathbf{x}^{(i)}) + (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top \mathbf{U}\mathbf{U}^\top (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}) \\ &= 0 \end{aligned}$$

# Pythagorean Theorem

The Pythagorean Theorem tells us:

$$\|\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}\|^2 + \|\mathbf{x}^{(i)} - \tilde{\mathbf{x}}^{(i)}\|^2 = \|\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}\|^2 \quad \text{for each } i$$

By averaging over data and from observation 2, we obtain



$$\begin{aligned} & \underbrace{\frac{1}{N} \sum_{i=1}^N \|\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}\|^2}_{\text{projected variance}} + \underbrace{\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}^{(i)} - \tilde{\mathbf{x}}^{(i)}\|^2}_{\text{reconstruction error}} \\ &= \underbrace{\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}\|^2}_{\text{constant}} \end{aligned}$$

Therefore,

projected variance = constant – reconstruction error

Maximizing the variance is equivalent to minimizing the reconstruction error!



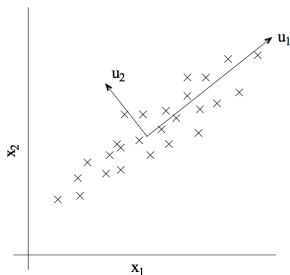
# Principal Component Analysis

Choosing a subspace to maximize the projected variance, or minimize the reconstruction error, is called **principal component analysis (PCA)**.

- Consider the **empirical covariance matrix**:

$$\hat{\Sigma} = \frac{1}{N} \sum_{i=1}^N (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top$$

- Recall:  $\hat{\Sigma}$  is symmetric and positive semidefinite.
- The optimal PCA subspace is spanned by the top  $K$  eigenvectors of  $\hat{\Sigma}$ .
  - ▶ More precisely, choose the first  $K$  of any orthonormal eigenbasis for  $\hat{\Sigma}$ .
  - ▶ The general case is tricky, but we'll show this for  $K = 1$ .
- These eigenvectors are called **principal components**, analogous to the principal axes of an ellipse.



## Supplement: Deriving PCA

- For  $K = 1$ , we are fitting a unit vector  $\mathbf{u}$ , and the code is a scalar  $z^{(i)} = \mathbf{u}^\top (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})$ . Let's maximize the projected variance. From observation 1, we have

$$\begin{aligned}\frac{1}{N} \sum_i \|\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}\|^2 &= \frac{1}{N} \sum_i [z^{(i)}]^2 = \frac{1}{N} \sum_i (\mathbf{u}^\top (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}))^2 \\ &= \frac{1}{N} \sum_{i=1}^N \mathbf{u}^\top (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}) (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top \mathbf{u} && (\mathbf{a}^\top \mathbf{b})^2 = \mathbf{a}^\top \mathbf{b} \mathbf{b}^\top \mathbf{a} \\ &= \mathbf{u}^\top \left[ \frac{1}{N} \sum_{i=1}^N (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}) (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top \right] \mathbf{u} \\ &= \mathbf{u}^\top \hat{\boldsymbol{\Sigma}} \mathbf{u} \\ &= \mathbf{u}^\top \mathbf{Q} \boldsymbol{\Lambda} \mathbf{Q}^\top \mathbf{u} && \text{Spectral Decomposition } \hat{\boldsymbol{\Sigma}} = \mathbf{Q} \boldsymbol{\Lambda} \mathbf{Q}^\top \\ &= \mathbf{a}^\top \boldsymbol{\Lambda} \mathbf{a} && \text{for } \mathbf{a} = \mathbf{Q}^\top \mathbf{u} \\ &= \sum_{j=1}^D \lambda_j a_j^2\end{aligned}$$

## Supplement: Deriving PCA

- Maximize  $\mathbf{a}^\top \mathbf{\Lambda} \mathbf{a} = \sum_{j=1}^D \lambda_j a_j^2$  for  $\mathbf{a} = \mathbf{Q}^\top \mathbf{u}$ .
  - ▶ This is a change-of-basis to the eigenbasis of  $\mathbf{\Sigma}$ .
- Assume the  $\lambda_i$  are in sorted order,  $\lambda_1 \geq \lambda_2, \geq \dots$
- Observation: since  $\mathbf{u}$  is a unit vector, then by unitarity,  $\mathbf{a}$  is also a unit vector:  $\mathbf{a}^\top \mathbf{a} = \mathbf{u}^\top \mathbf{Q} \mathbf{Q}^\top \mathbf{u} = \mathbf{u}^\top \mathbf{u}$ , i.e.,  $\sum_j a_j^2 = 1$ .
- By inspection, set  $a_1 = \pm 1$  and  $a_j = 0$  for  $j \neq 1$ .
- Hence,  $\mathbf{u} = \mathbf{Q} \mathbf{a} = \mathbf{q}_1$  (the top eigenvector).
  
- A similar argument shows that the  $k$ th principal component is the  $k$ th eigenvector of  $\mathbf{\Sigma}$ .

# Decorrelation

- Interesting fact: the dimensions of  $\mathbf{z}$  are decorrelated. For now, let  $\text{Cov}$  denote the empirical covariance.

$$\begin{aligned}\text{Cov}(\mathbf{z}) &= \text{Cov}(\mathbf{U}^\top (\mathbf{x} - \boldsymbol{\mu})) \\ &= \mathbf{U}^\top \text{Cov}(\mathbf{x}) \mathbf{U} \\ &= \mathbf{U}^\top \boldsymbol{\Sigma} \mathbf{U} \\ &= \mathbf{U}^\top \mathbf{Q} \boldsymbol{\Lambda} \mathbf{Q}^\top \mathbf{U} && \triangleright \text{spectral decomposition} \\ &= (\mathbf{I} \quad \mathbf{0}) \boldsymbol{\Lambda} \begin{pmatrix} \mathbf{I} \\ \mathbf{0} \end{pmatrix} && \triangleright \text{by orthogonality} \\ &= \text{top left } K \times K \text{ block of } \boldsymbol{\Lambda}\end{aligned}$$

- If the covariance matrix is diagonal, this means the features are uncorrelated.

Recap:

- Dimensionality reduction aims to find a low-dimensional representation of the data.
- PCA projects the data onto a subspace which maximizes the projected variance, or equivalently, minimizes the reconstruction error.
- The optimal subspace is given by the top eigenvectors of the empirical covariance matrix.
- PCA gives a set of decorrelated features.

# Applying PCA to faces

- Consider running PCA on 2429 19x19 grayscale images (CBCL data)
- Can get good reconstructions with only 3 components



- PCA for pre-processing: can apply classifier to latent representation
  - ▶ Original data is 361 dimensional
  - ▶ For face recognition PCA with 3 components obtains 79% accuracy on face/non-face discrimination on test data vs. 76.8% for a Gaussian mixture model (GMM) with 84 states. (We'll cover GMMs later in the course.)
- Can also be good for visualization

# Applying PCA to faces: Learned basis

Principal components of face images (“eigenfaces”)



# Applying PCA to digits



reconstructed with 2 bases



reconstructed with 10 bases



reconstructed with 100 bases



reconstructed with 506 bases



mean



principal basis 1



principal basis 2



principal basis 3





Two more interpretations of PCA, which have interesting generalizations.

1. **Matrix factorization**
2. Autoencoder














# Some recommender systems in action

The image shows a screenshot of the Netflix website interface. At the top, the Netflix logo is on the left, and navigation links for Home, TV Shows, Movies, Recently Added, and My List are in the center. On the right, there are icons for search, DVD, a notification bell, and a profile picture. Below the navigation bar, the 'Comedies' section is displayed with a row of movie posters: Kung Fu Panda 3, Disney Pixar Cars, The Land of Steady Habits, Downsizing, and To All the Boys I've Loved Before. The 'Top Picks for Juan Felipe' section follows with posters for The Wiggles Ready, Steady, Wiggle!, a man in a forest, SpongeBob SquarePants, Max & Ruby, and Transformers Rescue Bots. The 'Feel-good Animation' section at the bottom features posters for Mama Bear, Llama Llama, Barbie & the Great Escape Adventures, VeggieTales in the House, and Super Wings.

# The Netflix problem

Movie recommendation: Users watch movies and rate them out of 5★.

User	Movie	Rating
	Thor	★ ☆ ☆ ☆ ☆
	Chained	★ ★ ☆ ☆ ☆
	Frozen	★ ★ ★ ☆ ☆
	Chained	★ ★ ★ ★ ☆
	Bambi	★ ★ ★ ★ ★
	Titanic	★ ★ ★ ☆ ☆
	Goodfellas	★ ★ ★ ★ ★
	Dumbo	★ ★ ★ ★ ★
	Twilight	★ ★ ☆ ☆ ☆
	Frozen	★ ★ ★ ★ ★
	Tangled	★ ☆ ☆ ☆ ☆

Because users only rate a few items, one would like to infer their preference for unrated items

# Netflix Prize



# PCA as Matrix Factorization

- Recall PCA: each input vector  $\mathbf{x}^{(i)} \in \mathbb{R}^D$  is approximated as  $\hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{z}^{(i)}$ ,

$$\mathbf{x}^{(i)} \approx \tilde{\mathbf{x}}^{(i)} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{z}^{(i)}$$

where  $\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_i \mathbf{x}^{(i)}$  is the data mean,  $\mathbf{U} \in \mathbb{R}^{D \times K}$  is the orthogonal basis for the principal subspace, and  $\mathbf{z}^{(i)} \in \mathbb{R}^K$  is the code vector, and  $\tilde{\mathbf{x}}^{(i)} \in \mathbb{R}^D$  is  $\mathbf{x}^{(i)}$ 's reconstruction or approximation.

- Assume for simplicity that the data is centered:  $\hat{\boldsymbol{\mu}} = \mathbf{0}$ . Then, the approximation looks like

$$\mathbf{x}^{(i)} \approx \tilde{\mathbf{x}}^{(i)} = \mathbf{U}\mathbf{z}^{(i)}.$$

# PCA as Matrix Factorization

- PCA (on centered data): input vector  $\mathbf{x}^{(i)}$  is approximated as  $\mathbf{U}\mathbf{z}^{(i)}$

$$\mathbf{x}^{(i)} \approx \mathbf{U}\mathbf{z}^{(i)}$$

- Write this in matrix form, we have  $\mathbf{X} \approx \mathbf{Z}\mathbf{U}^\top$  where  $\mathbf{X}$  and  $\mathbf{Z}$  are matrices with one *row* per data point

$$\mathbf{X} = \begin{bmatrix} [\mathbf{x}^{(1)}]^\top \\ [\mathbf{x}^{(2)}]^\top \\ \vdots \\ [\mathbf{x}^{(N)}]^\top \end{bmatrix} \in \mathbb{R}^{N \times D} \quad \text{and} \quad \mathbf{Z} = \begin{bmatrix} [\mathbf{z}^{(1)}]^\top \\ [\mathbf{z}^{(2)}]^\top \\ \vdots \\ [\mathbf{z}^{(N)}]^\top \end{bmatrix} \in \mathbb{R}^{N \times K}$$

- Can write the squared reconstruction error as

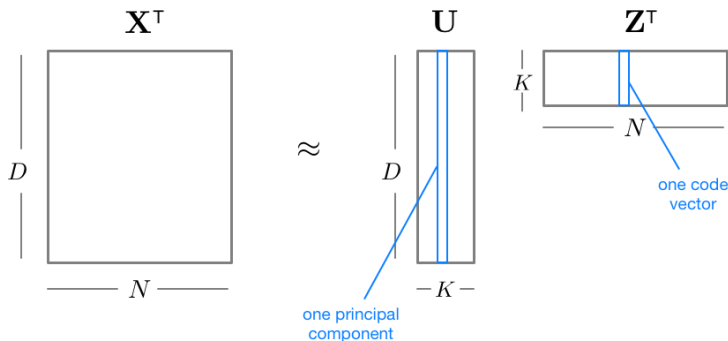
$$\sum_{i=1}^N \|\mathbf{x}^{(i)} - \mathbf{U}\mathbf{z}^{(i)}\|^2 = \|\mathbf{X} - \mathbf{Z}\mathbf{U}^\top\|_F^2,$$

- $\|\cdot\|_F$  denotes the **Frobenius norm**:

$$\|\mathbf{Y}\|_F^2 = \|\mathbf{Y}^\top\|_F^2 = \sum_{i,j} y_{ij}^2 = \sum_i \|\mathbf{y}^{(i)}\|^2.$$

# PCA as Matrix Factorization

- So PCA is approximating  $\mathbf{X} \approx \mathbf{Z}\mathbf{U}^\top$ , or equivalently  $\mathbf{X}^\top \approx \mathbf{U}\mathbf{Z}^\top$ .



- Based on the sizes of the matrices, this is a rank- $K$  approximation.
- Since  $\mathbf{U}$  was chosen to minimize reconstruction error, this is the *optimal* rank- $K$  approximation, in terms of error  $\|\mathbf{X}^\top - \mathbf{U}\mathbf{Z}^\top\|_F^2$ .



## PCA vs. SVD

This has a close relationship to the [Singular Value Decomposition \(SVD\)](#) of  $\mathbf{X}$ . This is a factorization

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$


Properties:

- $\mathbf{U}$ ,  $\mathbf{\Sigma}$ , and  $\mathbf{V}^\top$  provide a real-valued matrix factorization of  $\mathbf{X}$ , an  $m \times n$  matrix.
- $\mathbf{U}$  is a  $m \times m$  matrix with orthonormal columns  $\mathbf{U}^\top \mathbf{U} = \mathbf{I}_m$ , where  $\mathbf{I}_m$  is the  $m \times m$  identity matrix.
- $\mathbf{V}$  is an orthonormal  $n \times n$  matrix,  $\mathbf{V}^\top \mathbf{V} = \mathbf{I}_n$ .
- $\mathbf{\Sigma}$  is a  $m \times n$  diagonal matrix, with non-negative singular values,  $\sigma_1, \sigma_2, \dots, \sigma_{\min\{m,n\}}$ , on the diagonal, where the singular values are conventionally ordered from largest to smallest.

It's possible to show that the first  $n$  singular vectors correspond to the first  $n$  principal components; more precisely,  $\mathbf{Z} = \mathbf{U}\mathbf{\Sigma}$

# PCA vs. SVD (optional)

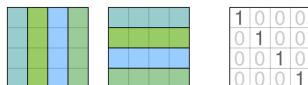
$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$



The diagram shows the decomposition of matrix  $\mathbf{M}$  into  $\mathbf{U}$ ,  $\mathbf{\Sigma}$ , and  $\mathbf{V}^*$ .  $\mathbf{M}$  is a 4x4 gray grid.  $\mathbf{U}$  is a 4x4 grid with columns colored teal, green, blue, and green.  $\mathbf{\Sigma}$  is a 4x4 grid with diagonal elements colored orange, yellow, yellow, and yellow, and zeros elsewhere.  $\mathbf{V}^*$  is a 4x4 grid with rows colored light blue, purple, purple, and pink.

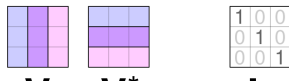
$$\mathbf{M} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^*$$

$m \times n$      $m \times m$      $m \times n$      $n \times n$



The diagram shows the decomposition of matrix  $\mathbf{U}$  into  $\mathbf{U}^*$  and  $\mathbf{I}_m$ .  $\mathbf{U}$  is a 4x4 grid with columns colored teal, green, blue, and green.  $\mathbf{U}^*$  is a 4x4 grid with rows colored green, green, blue, and green.  $\mathbf{I}_m$  is a 4x4 grid with diagonal elements colored 1 and zeros elsewhere.

$$\mathbf{U} \mathbf{U}^* = \mathbf{I}_m$$



The diagram shows the decomposition of matrix  $\mathbf{V}$  into  $\mathbf{V}^*$  and  $\mathbf{I}_n$ .  $\mathbf{V}$  is a 4x4 grid with columns colored light blue, purple, purple, and pink.  $\mathbf{V}^*$  is a 4x4 grid with rows colored light blue, purple, purple, and pink.  $\mathbf{I}_n$  is a 4x4 grid with diagonal elements colored 1 and zeros elsewhere.












$$\mathbf{V} \mathbf{V}^* = \mathbf{I}_n$$

# Matrix Completion

- We just saw that PCA gives the optimal low-rank matrix factorization to a matrix  $\mathbf{X}$ .
- Can we generalize this to the case where  $\mathbf{X}$  is only partially observed?
  - ▶ A sparse  $1000 \times 1000$  matrix with 50,000 observations (only 5% observed).
  - ▶ A rank 5 approximation requires only 10,000 parameters, so it's reasonable to fit this.
  - ▶ Unfortunately, no closed form solution.

# The Netflix problem

**Movie recommendation:** Users watch movies and rate them as good or bad.

User	Movie	Rating
	Thor	★ ☆ ☆ ☆ ☆
	Chained	★ ★ ☆ ☆ ☆
	Frozen	★ ★ ★ ☆ ☆
	Chained	★ ★ ★ ★ ☆
	Bambi	★ ★ ★ ★ ★
	Titanic	★ ★ ★ ☆ ☆
	Goodfellas	★ ★ ★ ★ ★
	Dumbo	★ ★ ★ ★ ★
	Twilight	★ ★ ☆ ☆ ☆
	Frozen	★ ★ ★ ★ ★
	Tangled	★ ☆ ☆ ☆ ☆

Because users only rate a few items, one would like to infer their preference for unrated items

# Matrix Completion

**Matrix completion problem:** Transform the table into a  $N$  users by  $M$  movies matrix  $\mathbf{R}$

Rating matrix

Ninja	2	3	?	?	?	?	?	1	?
Cat	4	?	5	?	?	?	?	?	?
Angel	?	?	?	3	5	5	?	?	?
Nursey	?	?	?	?	?	?	2	?	?
Tongey	?	5	?	?	?	?	?	?	?
Neutral	?	?	?	?	?	?	?	?	1
	Chained	Frozen	Bambi	Titanic	Goodfellas	Dumbo	Twilight	Thor	Tangled

- **Data:** Users rate some movies.  $\mathbf{R}_{\text{user},\text{movie}}$ . Very sparse
- **Task:** Predict missing entries, i.e. how a user would rate a movie they haven't previously rated
- **Evaluation Metric:** Squared error (used by Netflix Competition). Is this a reasonable metric?

# Matrix Completion

- In our current setting, **latent factor models** attempt to explain the ratings by characterizing both movies and users on a number of factors  $K$  inferred from the ratings patterns.
- That is, we seek representations for movies and users as vectors in  $\mathbb{R}^K$  that can ultimately be translated to ratings.
- For simplicity, we can associate these factors (i.e. the dimensions of the vectors) with idealized concepts like
  - ▶ comedy
  - ▶ drama
  - ▶ action
  - ▶ But also uninterpretable dimensions

Can we use the sparse ratings matrix  $\mathbf{R}$  to find these latent factors automatically?

# Matrix Completion

- Let the representation of user  $i$  in the  $K$ -dimensional space be  $\mathbf{u}_i$  and the representation of movie  $j$  be  $\mathbf{z}_j$ 
  - ▶ Intuition: maybe the first entry of  $\mathbf{u}_i$  says how much the user likes horror films, and the first entry of  $\mathbf{z}_j$  says how much movie  $j$  is a horror film.
- Assume the rating user  $i$  gives to movie  $j$  is given by a dot product:  
 $R_{ij} \approx \mathbf{u}_i^\top \mathbf{z}_j$
- In matrix form, if:

$$\mathbf{U} = \begin{bmatrix} - & \mathbf{u}_1^\top & - \\ & \vdots & \\ - & \mathbf{u}_N^\top & - \end{bmatrix} \text{ and } \mathbf{Z}^\top = \begin{bmatrix} | & & | \\ \mathbf{z}_1 & \dots & \mathbf{z}_M \\ | & & | \end{bmatrix}$$

then:  $\mathbf{R} \approx \mathbf{U}\mathbf{Z}^\top$

- This is a matrix factorization problem!

# Matrix Completion

- Recall PCA: To enforce  $\mathbf{X}^\top \approx \mathbf{U}\mathbf{Z}^\top$ , we minimized

$$\min_{\mathbf{U}, \mathbf{Z}} \|\mathbf{X}^\top - \mathbf{U}\mathbf{Z}^\top\|_F^2 = \sum_{i,j} (x_{ji} - \mathbf{u}_i^\top \mathbf{z}_j)^2$$

where  $\mathbf{u}_i$  and  $\mathbf{z}_i$  are the  $i$ -th rows of matrices  $\mathbf{U}$  and  $\mathbf{Z}$ , respectively.

- What's different about the Netflix problem?
  - ▶ Most entries are missing!
  - ▶ We only want to count the error for the observed entries.



# Matrix Completion

- Let  $O = \{(n, m) : \text{entry } (n, m) \text{ of matrix } \mathbf{R} \text{ is observed}\}$
- Using the squared error loss, matrix completion requires solving

$$\min_{\mathbf{U}, \mathbf{Z}} \frac{1}{2} \sum_{(i,j) \in O} (R_{ij} - \mathbf{u}_i^\top \mathbf{z}_j)^2$$

- The objective is non-convex in  $\mathbf{U}$  and  $\mathbf{Z}$  jointly, and in fact it's generally NP-hard to minimize the above cost function exactly.
- As a function of either  $\mathbf{U}$  or  $\mathbf{Z}$  individually, the problem is convex and easy to optimize. We can use coordinate descent, just like with K-means and mixture models!

**Alternating Least Squares (ALS):** fix  $\mathbf{Z}$  and optimize  $\mathbf{U}$ , followed by fix  $\mathbf{U}$  and optimize  $\mathbf{Z}$ , and so on until convergence.

# Alternating Least Squares

- Want to minimize the squared error cost with respect to the factor  $\mathbf{U}$ . (The case of  $\mathbf{Z}$  is exactly symmetric.)
- We can decompose the cost into a sum of independent terms:

$$\sum_{(i,j) \in O} \left( R_{ij} - \mathbf{u}_i^\top \mathbf{z}_j \right)^2 = \sum_i \underbrace{\sum_{j:(i,j) \in O} \left( R_{ij} - \mathbf{u}_i^\top \mathbf{z}_j \right)^2}_{\text{only depends on } \mathbf{u}_i}$$

This can be minimized independently for each  $\mathbf{u}_i$ .

- This is a linear regression problem in disguise. Its optimal solution is:

$$\mathbf{u}_i = \left( \sum_{j:(i,j) \in O} \mathbf{z}_j \mathbf{z}_j^\top \right)^{-1} \sum_{j:(i,j) \in O} R_{ij} \mathbf{z}_j$$

# Alternating Least Squares

ALS for Matrix Completion problem

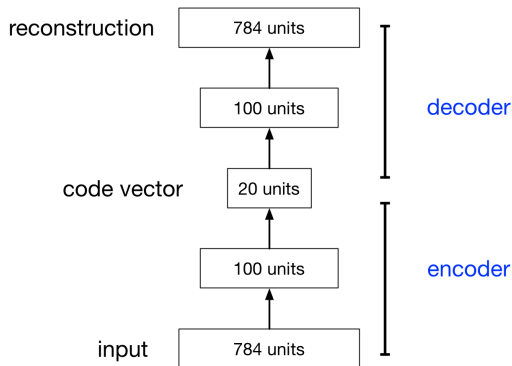
1. Initialize  $\mathbf{U}$  and  $\mathbf{Z}$  randomly
2. repeat until convergence
3.     **for**  $i = 1, \dots, N$  **do**
4.              $\mathbf{u}_i = \left( \sum_{j:(i,j) \in O} \mathbf{z}_j \mathbf{z}_j^\top \right)^{-1} \sum_{j:(i,j) \in O} R_{ij} \mathbf{z}_j$
5.     **for**  $j = 1, \dots, M$  **do**
6.              $\mathbf{z}_j = \left( \sum_{i:(i,j) \in O} \mathbf{u}_i \mathbf{u}_i^\top \right)^{-1} \sum_{i:(i,j) \in O} R_{ij} \mathbf{u}_i$

Two more interpretations of PCA, which have interesting generalizations.

1. Matrix factorization
2. **Autoencoder**

# Autoencoders

- An **autoencoder** is a feed-forward neural net whose job is to take an input  $\mathbf{x}$  and predict  $\mathbf{x}$ .
- To make this non-trivial, we need to add a **bottleneck layer** whose dimension is much smaller than the input.



# Linear Autoencoders

Why autoencoders?

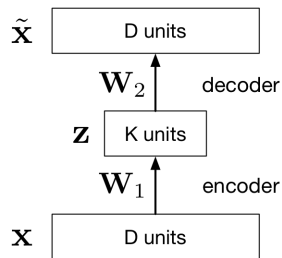
- Map high-dimensional data to two dimensions for visualization
- Learn abstract features in an unsupervised way so you can apply them to a supervised task
  - ▶ Unlabeled data can be much more plentiful than labeled data

# Linear Autoencoders

- The simplest kind of autoencoder has one hidden layer, linear activations, and squared error loss.

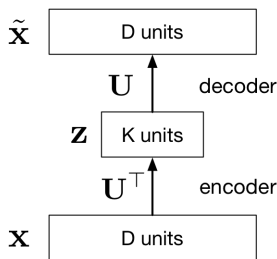
$$\mathcal{L}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|^2$$

- This network computes  $\tilde{\mathbf{x}} = \mathbf{W}_2 \mathbf{W}_1 \mathbf{x}$ , which is a linear function.
- If  $K \geq D$ , we can choose  $\mathbf{W}_2$  and  $\mathbf{W}_1$  such that  $\mathbf{W}_2 \mathbf{W}_1$  is the identity matrix. This isn't very interesting.
- But suppose  $K < D$ :
  - ▶  $\mathbf{W}_1$  maps  $\mathbf{x}$  to a  $K$ -dimensional space, so it's doing dimensionality reduction.



# Linear Autoencoders

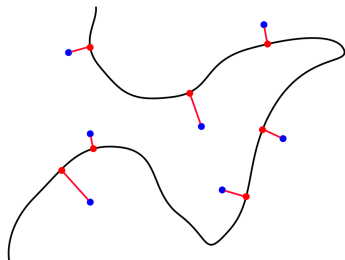
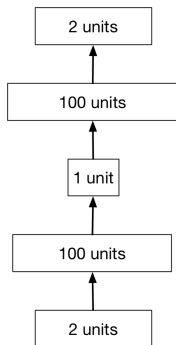
- Observe that the output of the autoencoder must lie in a  $K$ -dimensional subspace spanned by the columns of  $\mathbf{W}_2$ . This is because  $\tilde{\mathbf{x}} = \mathbf{W}_2\mathbf{z}$
- We saw that the best possible (min error)  $K$ -dimensional linear subspace in terms of reconstruction error is the PCA subspace.
- The autoencoder can achieve this by setting  $\mathbf{W}_1 = \mathbf{U}^\top$  and  $\mathbf{W}_2 = \mathbf{U}$ .
- Therefore, the optimal weights for a linear autoencoder are just the principal components!





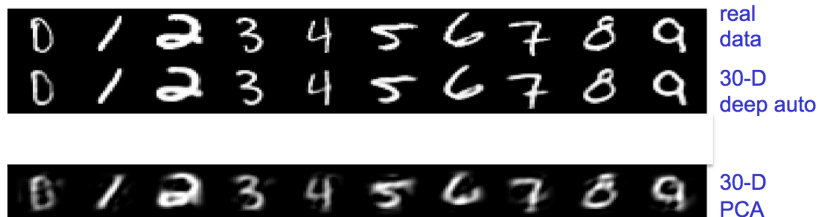
# Nonlinear Autoencoders

- Deep nonlinear autoencoders learn to project the data, not onto a subspace, but onto a nonlinear **manifold**
- This manifold is the image of the decoder.
- This is a kind of **nonlinear dimensionality reduction**.



# Nonlinear Autoencoders

- Nonlinear autoencoders can learn more powerful codes for a given dimensionality, compared with linear autoencoders (PCA)



# Nonlinear Autoencoders

Here's a 2-dimensional autoencoder representation of newsgroup articles. They're color-coded by topic, but the algorithm wasn't given the labels.

