

CSC 311: Introduction to Machine Learning

Lecture 10 - PCA, Matrix Completion, Autoencoders

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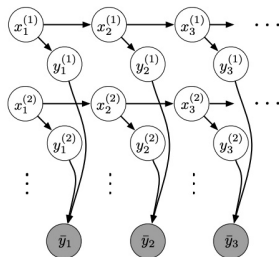
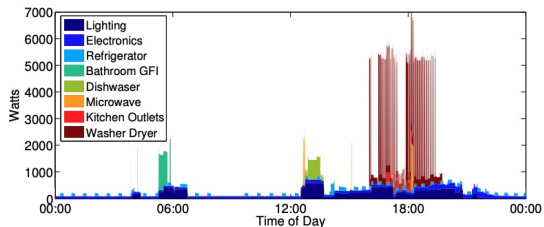
University of Toronto, Winter 2023

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

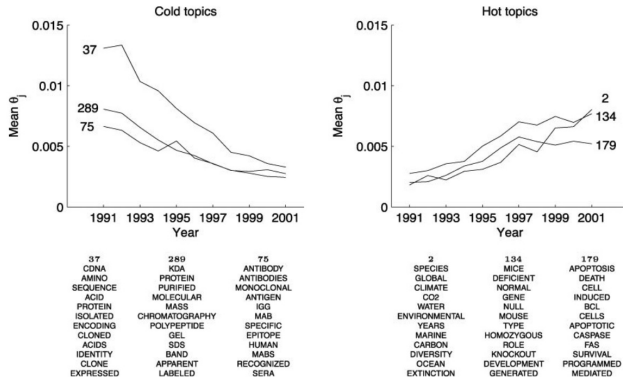
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|---|--|--|--|--|--|
| 217 INSECT MYB PHEROMONE LENS LARVAE | 274 SPECIES PHYLOGENETIC EVOLUTION EVOLUTIONARY SEQUENCES | 126 GENE VECTOR VECTORS EXPRESSION TRANSFER | 63 STRUCTURE ANGSTROM CRYSTAL RESIDUES STRUCTURES | 200 FOLDING NATIVE PROTEIN STATE 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 generalized¹ fundamental^{1,48} theorem²⁸⁷ of natural²⁵⁰ selection²⁵⁰ is derived²⁵¹ for populations²⁵⁰ incorporating^{1,49} both genetic²⁵⁰ and cultural²⁵⁰ transmission²⁵¹. The phenotype² is determined² by an arbitrary² number²⁷ of multiallelic² loci² with two⁷⁷-factor⁶⁹ epistasis²⁴⁰ and an arbitrary^{1,49} linkage² map², as well as by cultural¹⁵⁰ transmission²⁷ from the parents²⁵⁰. Generations²⁵⁰ are discrete⁶⁹ but partially²⁷ overlapping²⁵, and mating²⁵⁰ may be nonrandom²⁵⁰ at either the genotypic²⁵⁰ or the phenotypic²⁵⁰ level²⁵⁰ (or both). I show²⁷ that cultural¹⁵⁰ transmission²⁷ has several²⁷ important²⁷ implications²⁷ for the evolution²⁵⁰ of population¹⁵⁰ fitness²⁵⁰, most notably²¹⁰ that there is a time² lag² in the response²¹² to selection²⁵⁰ such that the future²⁷ evolution²⁵⁰ depends¹⁰⁷ on the past selection²⁵⁰ history²⁵⁰ of the population²⁵⁰.

Griffiths and Steyvers, "Finding scientific topics"

Motivating Examples

Modeling the change in scientific topics over time

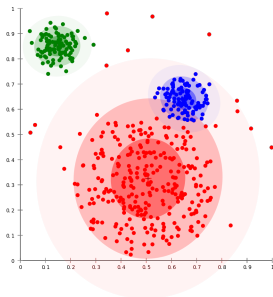


Griffiths and Steyvers, "Finding scientific topics"

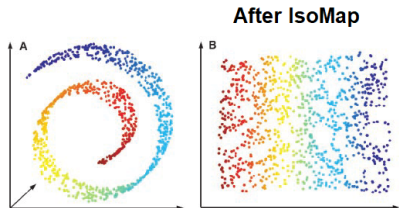
Motivating Examples

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**.

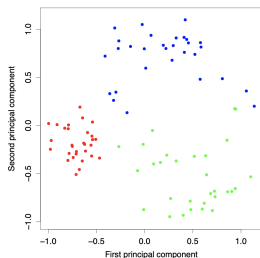
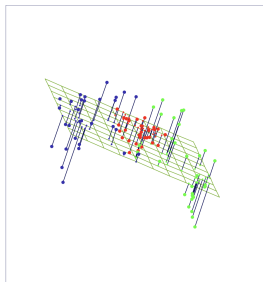
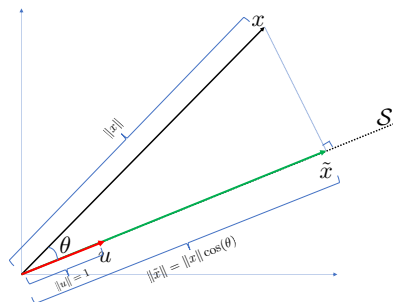


Image credit: Elements of Statistical Learning

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: $\mathbf{x}^T \mathbf{u} = \|\mathbf{x}\| \|\mathbf{u}\| \cos(\theta) = \|\mathbf{x}\| \cos(\theta)$
- $\text{Proj}_{\mathcal{S}}(\mathbf{x}) = \underbrace{\mathbf{x}^T \mathbf{u}}_{\text{length of proj}} \cdot \underbrace{\mathbf{u}}_{\text{direction of proj}} = \|\tilde{\mathbf{x}}\| \mathbf{u}$

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:

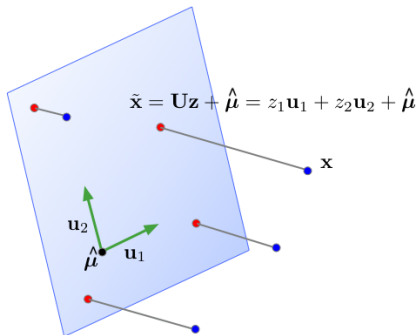
$$\text{Proj}_{\mathcal{S}}(\mathbf{x}) = \sum_{i=1}^K z_i \mathbf{u}_i \quad \text{where} \quad z_i = \mathbf{x}^\top \mathbf{u}_i.$$

- 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 $\hat{\boldsymbol{\mu}}$.

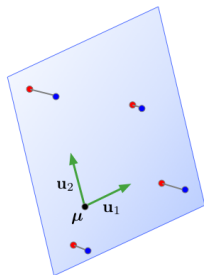


$$\mathbf{z} = \mathbf{U}^T(\mathbf{x} - \hat{\boldsymbol{\mu}})$$

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

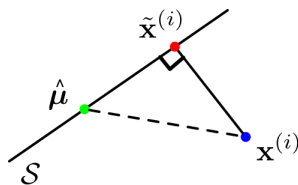
- **Observation 1:** Because the columns of \mathbf{U} are orthogonal, $\mathbf{U}^\top\mathbf{U} = \mathbf{I}$, so

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

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



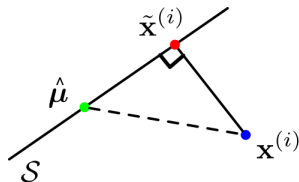
$$\begin{aligned} & (\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}})^\top (\tilde{\mathbf{x}}^{(i)} - \mathbf{x}^{(i)}) \\ &= (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top \mathbf{U}\mathbf{U}^\top (\hat{\boldsymbol{\mu}} - \mathbf{x}^{(i)} + \mathbf{U}\mathbf{U}^\top (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}))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

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,

$$\text{projected variance} = \text{constant} - \text{reconstruction error}$$

Maximizing the variance is equivalent to minimizing the reconstruction error!

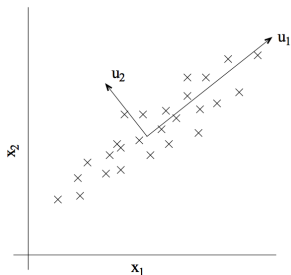
Principal Component Analysis

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.



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

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

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 λ_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 $\mathbf{\Sigma}$.

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 screenshot shows a browser window with the URL https://www.amazon.ca/?ref=_nav_signin&. The page displays a section titled "Inspired by your browsing history" with a "See more" link. Below this, there are seven book covers: "The Elements of Statistical Learning", "An Introduction to Statistical Learning", "DEEP LEARNING", "Hands On Machine Learning with Scikit-Learn & TensorFlow", "PATTERN RECOGNITION with MACHINE LEARNING", and "Machine Learning: A Probabilistic Perspective".

Below the books, there is a section titled "Your recently viewed items and featured recommendations" with a sub-header "Inspired by your browsing history". This section shows a carousel of seven items:

- Pixel 2 XL Case, Google Pixel 2 XL Case, Spigen Neo Hybrid - Flexible Inner TPU and Reinforced...** (4.5 stars, 134 reviews, CDN\$ 20.99 ✓prime)
- Pixel 2 XL Case, Google Pixel 2 XL Case, Spigen Thin Fit - Premium Matte Finish Coating for...** (4.5 stars, 143 reviews, CDN\$ 15.99 ✓prime)
- Google Pixel 2 XL Screen Protector [Not Glass][2-Pack], IQ Shield LiQuidSkin Full Coverage Screen Protector for Google...** (4.5 stars, 27.16 reviews, CDN\$ 27.16)
- Pixel 2 XL Case, Google Rugged Armor - Resilient Carbon Fiber Design...** (4.5 stars, 325 reviews, CDN\$ 15.99 ✓prime)
- VicTsing Mini DisplayPort (Thunderbolt Port Compatible) to HDMI/DVI/VGA Male to...** (4.5 stars, 306 reviews, CDN\$ 16.99 ✓prime)
- UGREEN Active Micro HDMI to HDMI VGA Video Converter Adapter with 3.5mm Audio Jack and...** (4.5 stars, 64 reviews, CDN\$ 25.49 ✓prime)
- AmazonBasics Nylon Braided USB A to Lightning Compatible Cable - Apple MFL...** (4.5 stars, 402 reviews, CDN\$ 12.99 ✓prime)

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Ideally recommendations should combine global and seasonal interests, look at your history if available, should adapt with time, be coherent and diverse, etc.

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, featuring 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 includes 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

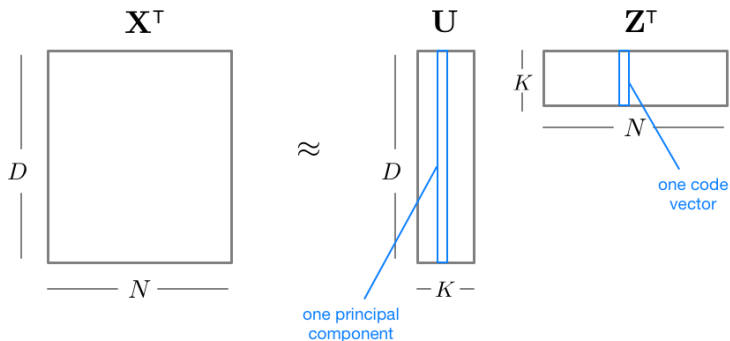
$$\sum_{i=1}^N \|\mathbf{x}^{(i)} - \mathbf{U}\mathbf{z}^{(i)}\|^2 = \|\mathbf{X} - \mathbf{Z}\mathbf{U}^\top\|_F^2,$$

- $\|\cdot\|_F$ 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

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


Properties:

- \mathbf{U} , $\mathbf{\Sigma}$, and \mathbf{V}^T 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 $\mathbf{U}^T \mathbf{U} = \mathbf{I}_m$, where \mathbf{I}_m is the $m \times m$ identity matrix.
- \mathbf{V} is an orthonormal $n \times n$ matrix, $\mathbf{V}^T \mathbf{V} = \mathbf{I}_n$.
- $\mathbf{\Sigma}$ 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)

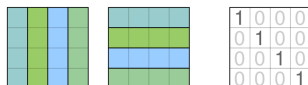
$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$



The diagram shows a 4x4 matrix \mathbf{M} (grey) being decomposed into a 4x4 matrix \mathbf{U} (green and blue columns), a 4x4 matrix $\mathbf{\Sigma}$ (diagonal with orange, yellow, and white blocks), and a 4x4 matrix \mathbf{V}^* (purple and pink rows).

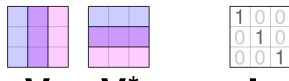
$$\mathbf{M} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^*$$

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



The diagram shows a 4x4 matrix \mathbf{U} (green and blue columns) being decomposed into a 4x4 matrix \mathbf{U}^* (green and blue rows) and a 4x4 identity matrix \mathbf{I}_m (diagonal with 1s).

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



The diagram shows a 4x4 matrix \mathbf{V} (purple and pink rows) being decomposed into a 4x4 matrix \mathbf{V}^* (purple and pink columns) and a 4x4 identity matrix \mathbf{I}_n (diagonal with 1s).












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

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 1000×1000 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

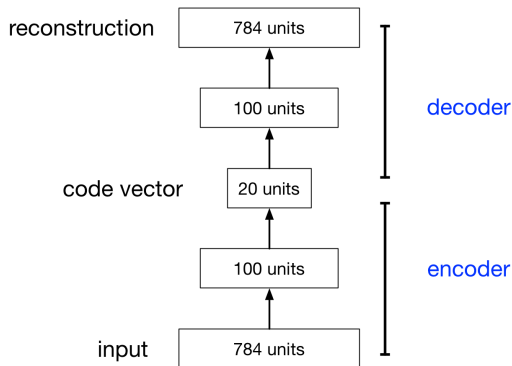
1. Initialize \mathbf{U} and \mathbf{Z} randomly
2. repeat until convergence
3. **for** $i = 1, \dots, N$ **do**
4. $\mathbf{u}_i = \left(\sum_{j:(i,j) \in O} \mathbf{z}_j \mathbf{z}_j^\top \right)^{-1} \sum_{j:(i,j) \in O} R_{ij} \mathbf{z}_j$
5. **for** $j = 1, \dots, M$ **do**
6. $\mathbf{z}_j = \left(\sum_{i:(i,j)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

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?

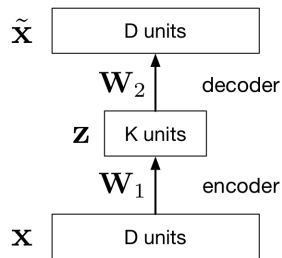
- Map high-dimensional data to two dimensions for visualization
- Learn abstract features in an unsupervised way so you can apply them to a supervised task
 - ▶ Unlabeled data can be much more plentiful than labeled data

Linear Autoencoders

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

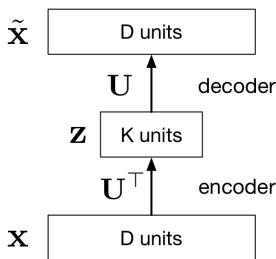
$$\mathcal{L}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|^2$$

- 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.



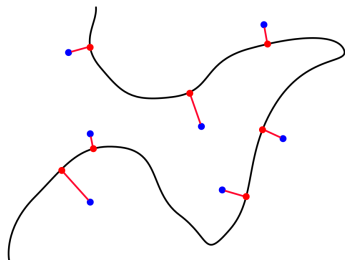
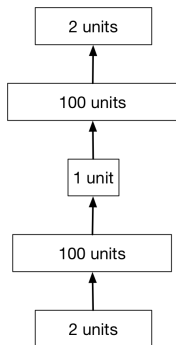
Linear Autoencoders

- 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!



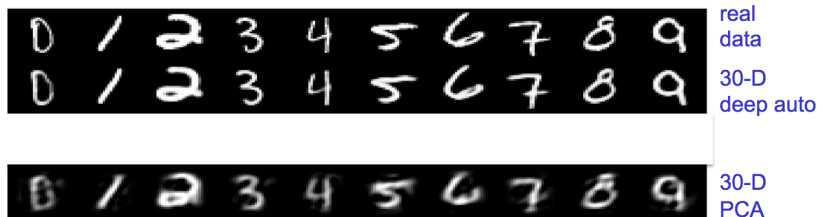
Nonlinear Autoencoders

- 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.

