CSC 311: Introduction to Machine Learning
Lecture 10 - PCA, Matrix Completion, Autoencoders

Rahul G. Krishnan    Alice Gao

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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

Griffiths and Steyvers, “Finding scientific topics”
Motivating Examples

Modeling the change in scientific topics over time

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

- How to project onto a $K$-dimensional subspace?
  - **Idea:** choose an orthonormal basis $\{u_1, u_2, \cdots, u_K\}$ for $S$ (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:

  $$\text{Proj}_S(x) = \sum_{i=1}^{K} z_i u_i \text{ where } z_i = x^\top u_i.$$ 

- In vector form:

  $$\text{Proj}_S(x) = Uz \text{ where } z = U^\top x$$
Projection onto a Subspace

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

\[ \tilde{x} = Uz + \hat{\mu} = z_1u_1 + z_2u_2 + \hat{\mu} \]

\[ z = U^T(x - \hat{\mu}) \]

- In machine learning, $\tilde{x}$ is also called the reconstruction of $x$.
- $z$ is its representation, or code.
Projection onto a Subspace

- If we have a $K$-dimensional subspace in a $D$-dimensional input space, then $x \in \mathbb{R}^D$ and $z \in \mathbb{R}^K$.
- If the data points $x$ all lie close to their reconstructions, then we can approximate distances, etc. in terms of these same operations on the code vectors $z$.
- If $K \ll D$, then it’s much cheaper to work with $z$ than $x$.
- 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 $\hat{\mu}$ is the empirical mean of the data
  - Need to choose a $D \times K$ matrix $U$ with orthonormal columns.

- Two criteria:
  - Minimize the reconstruction error:
    $$\min_U \frac{1}{N} \sum_{i=1}^{N} \| x^{(i)} - \tilde{x}^{(i)} \|^2$$
  - Maximize the variance of reconstructions: Find a subspace where data has the most variability.
    $$\max_U \frac{1}{N} \sum_{i} \| \tilde{x}^{(i)} - \hat{\mu} \|^2$$
  - Note: The data and its reconstruction have the same means (exercise)!
Learning a Subspace

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

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

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

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

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

$\implies$ norm of centered reconstruction is equal to norm of representation. (If you draw it, this is obvious).
Observation 1: \( \| \tilde{x}^{(i)} - \hat{\mu} \|^2 = \| z^{(i)} \|^2 \)
- Variance of reconstructions is equal to variance of code vectors:
  \[
  \frac{1}{N} \sum_i \| \tilde{x}^{(i)} - \hat{\mu} \|^2 = \frac{1}{N} \sum_i \| z^{(i)} \|^2 \quad \text{(exercise } \frac{1}{N} \sum_i z^{(i)} = 0)\]

Observation 2: orthogonality of \( \tilde{x}^{(i)} - \hat{\mu} \) and \( \tilde{x}^{(i)} - x^{(i)} \)
- (Two vectors \( \mathbf{a}, \mathbf{b} \) are orthogonal \( \iff \mathbf{a}^\top \mathbf{b} = 0 \))

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

\[
(\tilde{x}^{(i)} - \hat{\mu})^\top (\tilde{x}^{(i)} - x^{(i)}) \\
= (x^{(i)} - \hat{\mu})^\top \mathbf{U} \mathbf{U}^\top (\hat{\mu} - x^{(i)}) + \mathbf{U} \mathbf{U}^\top (x^{(i)} - \hat{\mu}) \\
= (x^{(i)} - \hat{\mu})^\top \mathbf{U} \mathbf{U}^\top (\hat{\mu} - x^{(i)}) + (x^{(i)} - \hat{\mu})^\top \mathbf{U} \mathbf{U}^\top (x^{(i)} - \hat{\mu}) \\
= 0
\]
The Pythagorean Theorem tells us:

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

By averaging over data and from observation 2, we obtain

\[
\frac{1}{N} \sum_{i=1}^{N} \|\tilde{x}^{(i)} - \hat{\mu}\|^2 + \frac{1}{N} \sum_{i=1}^{N} \|x^{(i)} - \tilde{x}^{(i)}\|^2
\]

\[
= \frac{1}{N} \sum_{i=1}^{N} \|x^{(i)} - \hat{\mu}\|^2
\]

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:
  \[
  \hat{\Sigma} = \frac{1}{N} \sum_{i=1}^{N} (x^{(i)} - \hat{\mu})(x^{(i)} - \hat{\mu})^\top
  \]

- 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 $z^{(i)} = \mathbf{u}^\top (\mathbf{x}^{(i)} - \hat{\mu})$. Let’s maximize the projected variance. From observation 1, we have

$$
\frac{1}{N} \sum_i \|\tilde{\mathbf{x}}^{(i)} - \hat{\mu}\|^2 = \frac{1}{N} \sum_i [z^{(i)}]^2 = \frac{1}{N} \sum_i (\mathbf{u}^\top (\mathbf{x}^{(i)} - \hat{\mu}))^2
$$

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

$$
= \mathbf{u}^\top \left[ \frac{1}{N} \sum_{i=1}^N (\mathbf{x}^{(i)} - \hat{\mu})(\mathbf{x}^{(i)} - \hat{\mu})^\top \right] \mathbf{u}
$$

$$
= \mathbf{u}^\top \hat{\Sigma} \mathbf{u}
$$

$$
= \mathbf{u}^\top \mathbf{Q}\Lambda\mathbf{Q}^\top \mathbf{u}
$$

Spectral Decomposition $\hat{\Sigma} = \mathbf{Q}\Lambda\mathbf{Q}^\top$

$$
= \mathbf{a}^\top \Lambda \mathbf{a}
$$

$$
= \sum_{j=1}^D \lambda_j a_j^2
$$
Supplement: Deriving PCA

- Maximize $\mathbf{a}^\top \Lambda \mathbf{a} = \sum_{j=1}^{D} \lambda_j a_j^2$ for $\mathbf{a} = Q^\top \mathbf{u}$.
  - This is a change-of-basis to the eigenbasis of $\Sigma$.
- Assume the $\lambda_i$ are in sorted order, $\lambda_1 \geq \lambda_2, \geq ...$
- Observation: since $\mathbf{u}$ is a unit vector, then by unitarity, $\mathbf{a}$ is also a unit vector: $\mathbf{a}^\top \mathbf{a} = \mathbf{u}^\top QQ^\top \mathbf{u} = \mathbf{u}^\top \mathbf{u}$, i.e., $\sum_j a_j^2 = 1$.
- By inspection, set $a_1 = \pm 1$ and $a_j = 0$ for $j \neq 1$.
- Hence, $\mathbf{u} = Q\mathbf{a} = q_1$ (the top eigenvector).

- A similar argument shows that the $k$th principal component is the $k$th eigenvector of $\Sigma$. 
Interesting fact: the dimensions of $\mathbf{z}$ are decorrelated. For now, let $\text{Cov}$ denote the empirical covariance.

$$
\text{Cov}(\mathbf{z}) = \text{Cov}(\mathbf{U}^\top (\mathbf{x} - \mathbf{\mu}))
$$

$$
= \mathbf{U}^\top \text{Cov}(\mathbf{x}) \mathbf{U}
$$

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

$$
= \mathbf{U}^\top \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top \mathbf{U}
\quad \triangleright \text{ spectral decomposition}
$$

$$
= (\mathbf{I} \quad 0) \mathbf{\Lambda} \begin{pmatrix} \mathbf{I} \\ 0 \end{pmatrix}
\quad \triangleright \text{ by orthogonality}
$$

$$
= \text{top left } K \times K \text{ block of } \mathbf{\Lambda}
$$

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

![Faces images]

- 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

3 3 3 3 3 3
3 3 3 3 3 3
3 3 3 3 3 3
3 3 3 3 3 3
3 3 3 3 3 3
3 3 3 3 3 3
mean
principal basis 1
principal basis 2
principal basis 3
reconstructed with 2 bases
reconstructed with 10 bases
reconstructed with 100 bases
reconstructed with 506 bases
Two more interpretations of PCA, which have interesting generalizations.

1. **Matrix factorization**
2. **Autoencoder**
Some recommender systems in action

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 Netflix problem

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

<table>
<thead>
<tr>
<th>User</th>
<th>Movie</th>
<th>Rating</th>
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</thead>
<tbody>
<tr>
<td>🎥</td>
<td>Thor</td>
<td>⭐⭐⭐⭐⭐</td>
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<td>🎥</td>
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Because users only rate a few items, one would like to infer their preference for unrated items.
Netflix Prize

PAY TO THE ORDER OF: BellKor's Pragmatic Chaos

AMOUNT: ONE MILLION

FOR: The Netflix Prize

Date: 09.21.09

The Netflix Prize
Recall PCA: each input vector $\mathbf{x}^{(i)} \in \mathbb{R}^D$ is approximated as

$$\hat{\mu} + \mathbf{U} \mathbf{z}^{(i)},$$

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

where $\hat{\mu} = \frac{1}{n} \sum_i \mathbf{x}^{(i)}$ 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: $\hat{\mu} = 0$. 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 $\mathbf{Uz}^{(i)}$
  \[ \mathbf{x}^{(i)} \approx \mathbf{Uz}^{(i)} \]

- Write this in matrix form, we have $\mathbf{X} \approx \mathbf{ZU}^\top$ 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
  \[ \sum_{i=1}^{N} \| \mathbf{x}^{(i)} - \mathbf{Uz}^{(i)} \|^2 = \| \mathbf{X} - \mathbf{ZU}^\top \|^2_F, \]

- $\| \cdot \|_F$ denotes the Frobenius norm:
  \[ \| \mathbf{Y} \|^2_F = \| \mathbf{Y}^\top \|^2_F = \sum_{i,j} y_{ij}^2 = \sum_{i} \| \mathbf{y}^{(i)} \|^2. \]
So PCA is approximating $X \approx ZU^\top$, or equivalently $X^\top \approx UZ^\top$.

Based on the sizes of the matrices, this is a rank-$K$ approximation.

Since $U$ was chosen to minimize reconstruction error, this is the *optimal* rank-$K$ approximation, in terms of error $\|X^\top - UZ^\top\|_F^2$. 
PCA vs. SVD

This has a close relationship to the Singular Value Decomposition (SVD) of $X$. This is a factorization

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

Properties:

- $U$, $\Sigma$, and $V^\top$ provide a real-valued matrix factorization of $X$, an $m \times n$ matrix.
- $U$ is a $m \times m$ matrix with orthonormal columns $U^\top U = I_m$, where $I_m$ is the $m \times m$ identity matrix.
- $V$ is an orthonormal $n \times n$ matrix, $V^\top V = I_n$.
- $\Sigma$ is a $m \times n$ diagonal matrix, with non-negative singular values, $\sigma_1, \sigma_2, \ldots, \sigma_{\min\{m,n\}}$, 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, $Z = U \Sigma$
PCA vs. SVD (optional)

\[ X = U \Sigma V^T \]

\[ M_{m \times n} = U_{m \times m} \Sigma_{m \times n} V^*_{n \times n} \]

\[ U U^* = I_m \]

\[ V V^* = I_n \]
Matrix Completion

- We just saw that PCA gives the optimal low-rank matrix factorization to a matrix $X$.
- Can we generalize this to the case where $X$ 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.

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Because users only rate a few items, one would like to infer their preference for unrated items.
Matrix completion problem: Transform the table into a $N$ users by $M$ movies matrix $R$.

- **Data**: Users rate some movies. $R_{user, movie}$. 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 $u_i$ and the representation of movie $j$ be $z_j$.
  - Intuition: maybe the first entry of $u_i$ says how much the user likes horror films, and the first entry of $z_j$ says how much movie $j$ is a horror film.
- Assume the rating user $i$ gives to movie $j$ is given by a dot product: $R_{ij} \approx u_i^T z_j$
- In matrix form, if:
  $$U = \begin{bmatrix} - & u_1^T & - \\ - & \vdots & - \\ - & u_N^T & - \end{bmatrix} \quad \text{and} \quad Z^T = \begin{bmatrix} | & | & | \\ z_1 & \cdots & z_M \end{bmatrix}$$
  then: $R \approx UZ^T$
- This is a matrix factorization problem!
Matrix Completion

- Recall PCA: To enforce $X^\top \approx UZ^\top$, we minimized
  \[
  \min_{U,Z} \|X^\top - UZ^\top\|_F^2 = \sum_{i,j} (x_{ji} - u_i^\top z_j)^2
  \]
  where $u_i$ and $z_i$ are the $i$-th rows of matrices $U$ and $Z$, 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 \( O = \{(n, m) : \text{entry } (n, m) \text{ of matrix } R \text{ is observed}\} \)

Using the squared error loss, matrix completion requires solving

\[
\min_{U,Z} \frac{1}{2} \sum_{(i,j) \in O} \left( R_{ij} - u_i^T z_j \right)^2
\]

The objective is non-convex in \( U \) and \( Z \) jointly, and in fact it’s generally NP-hard to minimize the above cost function exactly.

As a function of either \( U \) or \( Z \) 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 \( Z \) and optimize \( U \), followed by fix \( U \) and optimize \( Z \), and so on until convergence.
Alternating Least Squares

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

$$\sum_{(i,j) \in O} \left( R_{ij} - u_i^T z_j \right)^2 = \sum_i \left( R_{ij} - u_i^T z_j \right)^2$$

This can be minimized independently for each $u_i$.
- This is a linear regression problem in disguise. Its optimal solution is:

$$u_i = \left( \sum_{j: (i,j) \in O} z_j z_j^T \right)^{-1} \sum_{j: (i,j) \in O} R_{ij} z_j$$
ALS for Matrix Completion problem

1. Initialize $U$ and $Z$ randomly

2. repeat until convergence

3. for $i = 1, \ldots, N$ do

4. $u_i = \left( \sum_{j:(i,j) \in O} z_j z_j^\top \right)^{-1} \sum_{j:(i,j) \in O} R_{ij} z_j$

5. for $j = 1, \ldots, M$ do

6. $z_j = \left( \sum_{i:(i,j) \in O} u_i u_i^\top \right)^{-1} \sum_{i:(i,j) \in O} R_{ij} u_i$
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.
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.

\[ \mathcal{L}(x, \tilde{x}) = \| x - \tilde{x} \|^2 \]

- This network computes \( \tilde{x} = W_2 W_1 x \), which is a linear function.

- If \( K \geq D \), we can choose \( W_2 \) and \( W_1 \) such that \( W_2 W_1 \) is the identity matrix. This isn’t very interesting.

- But suppose \( K < D \):
  - \( W_1 \) maps \( x \) 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 $W_2$. This is because $\tilde{x} = W_2z$
- 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 $W_1 = U^\top$ and $W_2 = U$.
- Therefore, the optimal weights for a linear autoencoder are just the principal components!

![Diagram of linear autoencoder](image)

\[ \tilde{x} \quad \text{D units} \]

\[ U \quad \text{decoder} \]

\[ Z \quad \text{K units} \]

\[ U^\top \quad \text{encoder} \]

\[ x \quad \text{D units} \]
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.