CSC 311: Introduction to Machine Learning

Lecture 9 - PCA cont'd, Autoencoders, Matrix Factorization

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Today

- Finishing Principal Component Analysis (PCA)
  - Last time: key linear algebra concepts, overview of the algorithm itself
  - Today: why the algorithm works
- Two generalizations of PCA
  - Matrix completion
  - Autoencoders

Recap: PCA

- Summarize data by projecting onto a low-dimensional subspace

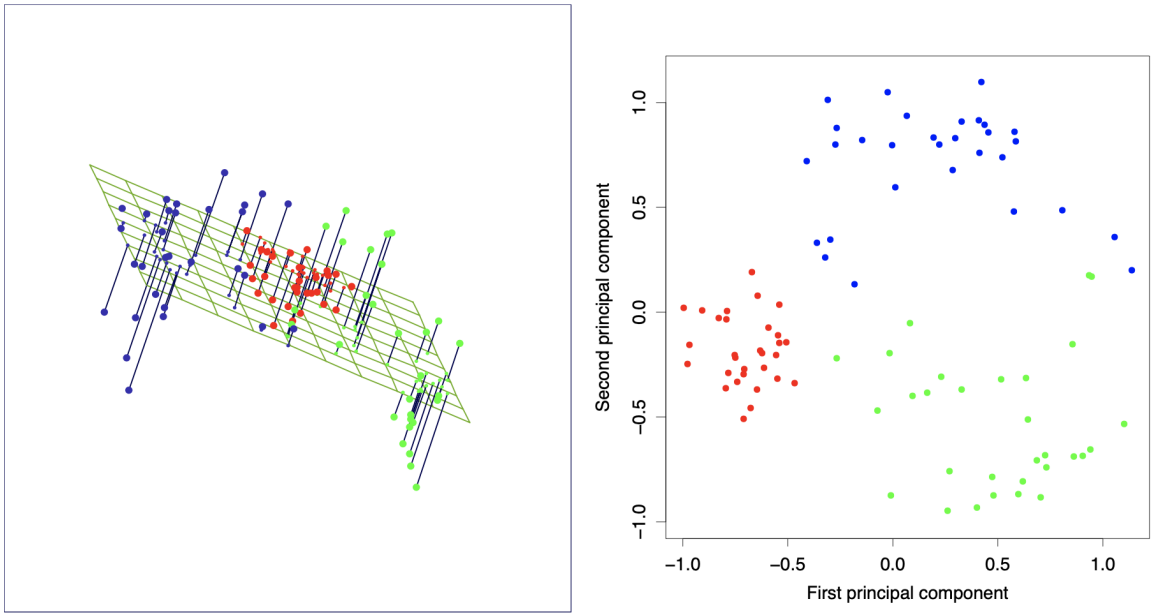
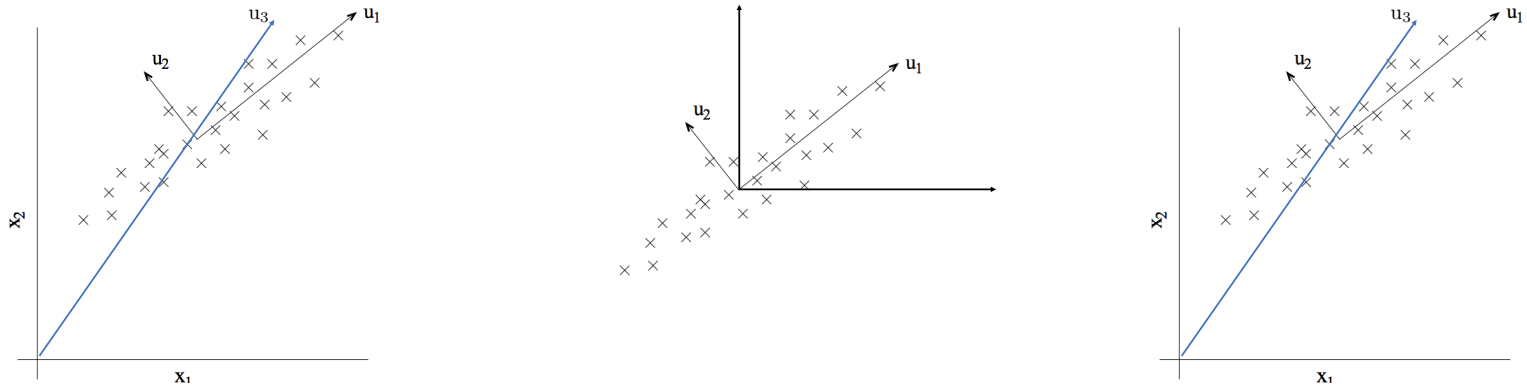


Image credit: Elements of Statistical Learning

- Some benefits of a low-dimensional representation
  - Reduce memory and computation costs
  - Interpretability, visualization
  - Generalization

Recap: PCA



Summary for a given point $\mathbf{x}$:

1. Subtract mean: $\mathbf{x} - \hat{\boldsymbol{\mu}}$
2. Project on $\mathcal{S}$: $\mathbf{U}\mathbf{U}^\top(\mathbf{x} - \hat{\boldsymbol{\mu}})$, where columns of $\mathbf{U}$ are unit eigenvectors for largest K eigenvalues of $\hat{\boldsymbol{\Sigma}}$ (K directions of highest variance)
3. Add back mean: $\hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{U}^\top(\mathbf{x} - \hat{\boldsymbol{\mu}})$

The reconstruction is $\tilde{\mathbf{x}} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{z} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{U}^T(\mathbf{x} - \hat{\boldsymbol{\mu}})$

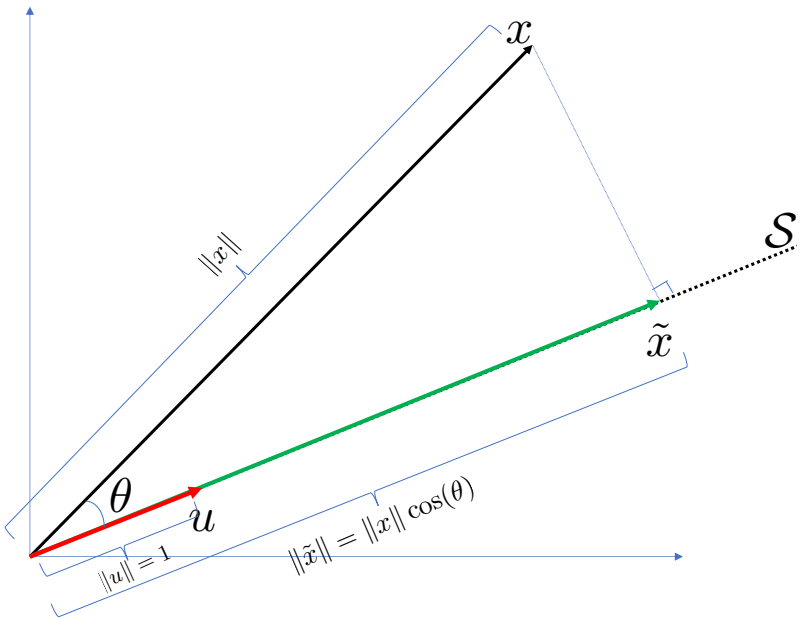
Here, $\mathbf{z} = \mathbf{U}^T(\mathbf{x} - \hat{\boldsymbol{\mu}})$ is a lower dimensional representation of $\mathbf{x}$.

And that's it! We've done Principal Component Analysis (PCA)!

- Let's now do this again in a bit more detail...

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 $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_K\}$ 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:

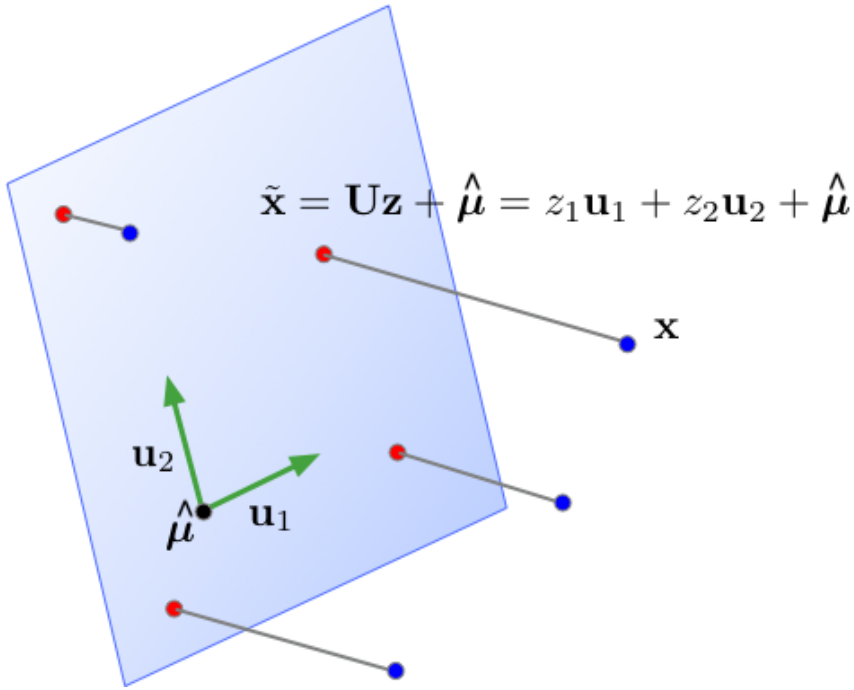
$$\text{Proj}_{\mathcal{S}}(\mathbf{x}) = \sum_{i=1}^{K} z_i \mathbf{u}_i \quad \text{where} \quad z_i = \mathbf{x}^\top \mathbf{u}_i.$$

- In vector form:

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

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

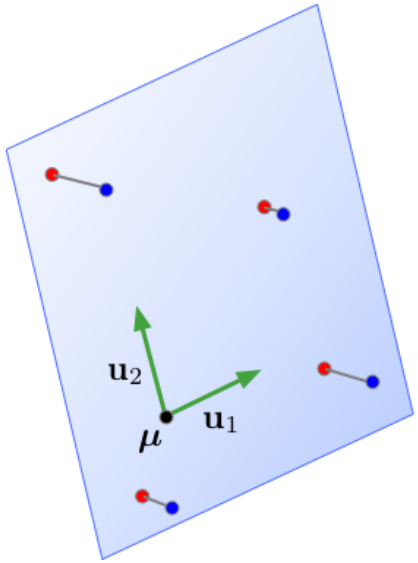


$$\mathbf{z} = \mathbf{U}^\top(\mathbf{x} - \hat{\boldsymbol{\mu}})$$

- 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

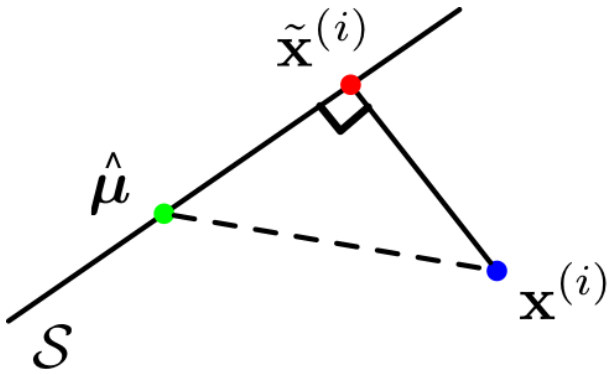
$$\|\tilde{\mathbf{x}}-\hat{\boldsymbol{\mu}}\|^2 = \|\mathbf{U}\mathbf{z}\|^2 = \mathbf{z}^\top\mathbf{U}^\top\mathbf{U}\mathbf{z} = \mathbf{z}^\top\mathbf{z} = \|\mathbf{z}\|^2.$$

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



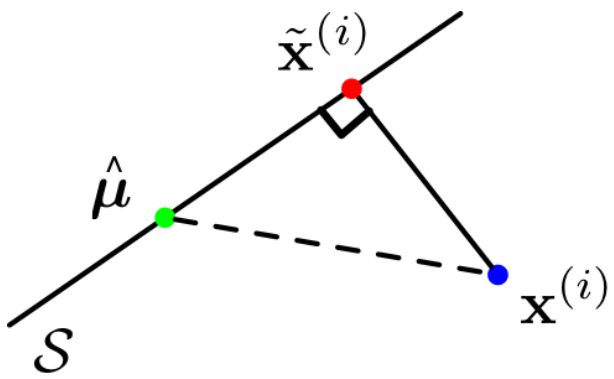
$$
\begin{aligned}
&(\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}})^\top(\tilde{\mathbf{x}}^{(i)} - \mathbf{x}^{(i)}) \\
&= (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top \mathbf{U}\mathbf{U}^\top(\hat{\boldsymbol{\mu}} - \mathbf{x}^{(i)} + \mathbf{U}\mathbf{U}^\top(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}))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

Pythagorean Theorem

The Pythagorean Theorem tells us:

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

By averaging over data and from observation 2, we obtain



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

$$= \underbrace{\frac{1}{N}\sum_{i=1}^{N}\|\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}\|^2}_{\text{constant}}$$

Therefore,

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

Maximizing the variance is equivalent to minimizing the reconstruction error!

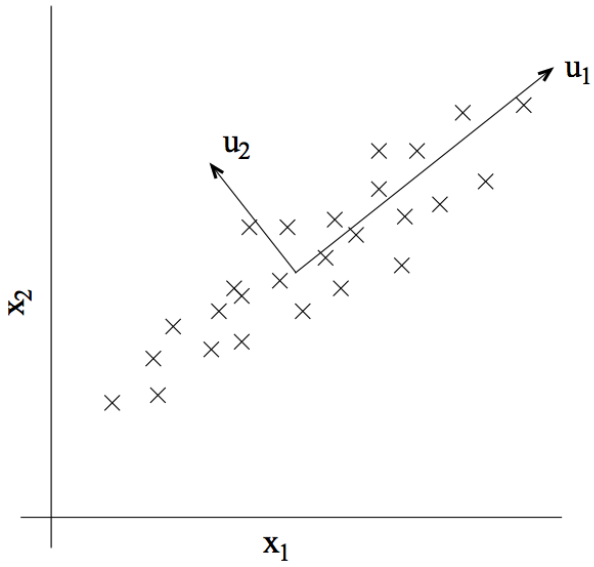
Principal Component Analysis

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

- Consider the empirical covariance matrix:

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

- Recall: $\hat{\boldsymbol{\Sigma}}$ is symmetric and positive semidefinite.
- The optimal PCA subspace is spanned by the top K eigenvectors of $\hat{\boldsymbol{\Sigma}}$.
  - More precisely, choose the first K of any orthonormal eigenbasis for $\hat{\boldsymbol{\Sigma}}$.
  - 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

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

$$= \frac{1}{N}\sum_{i=1}^N \mathbf{u}^\top(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^\top\mathbf{u} \qquad (\mathbf{a}^\top\mathbf{b})^2 = \mathbf{a}^\top\mathbf{b}\mathbf{b}^\top\mathbf{a}$$

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

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

$$= \mathbf{u}^\top\mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\top\mathbf{u} \qquad \text{Spectral Decomposition } \hat{\boldsymbol{\Sigma}} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\top$$

$$= \mathbf{a}^\top\boldsymbol{\Lambda}\mathbf{a} \qquad \text{for } \mathbf{a} = \mathbf{Q}^\top\mathbf{u}$$

$$= \sum_{j=1}^D \lambda_j a_j^2$$

Supplement: Deriving PCA

- Maximize $\mathbf{a}^\top \mathbf{\Lambda a} = \sum_{j=1}^{D} \lambda_j a_j^2$ 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, $\lambda_1 \geq \lambda_2, \geq \ldots$
- 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 kth principal component is the kth eigenvector of $\mathbf{\Sigma}$.

Decorrelation

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

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

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

Recap

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

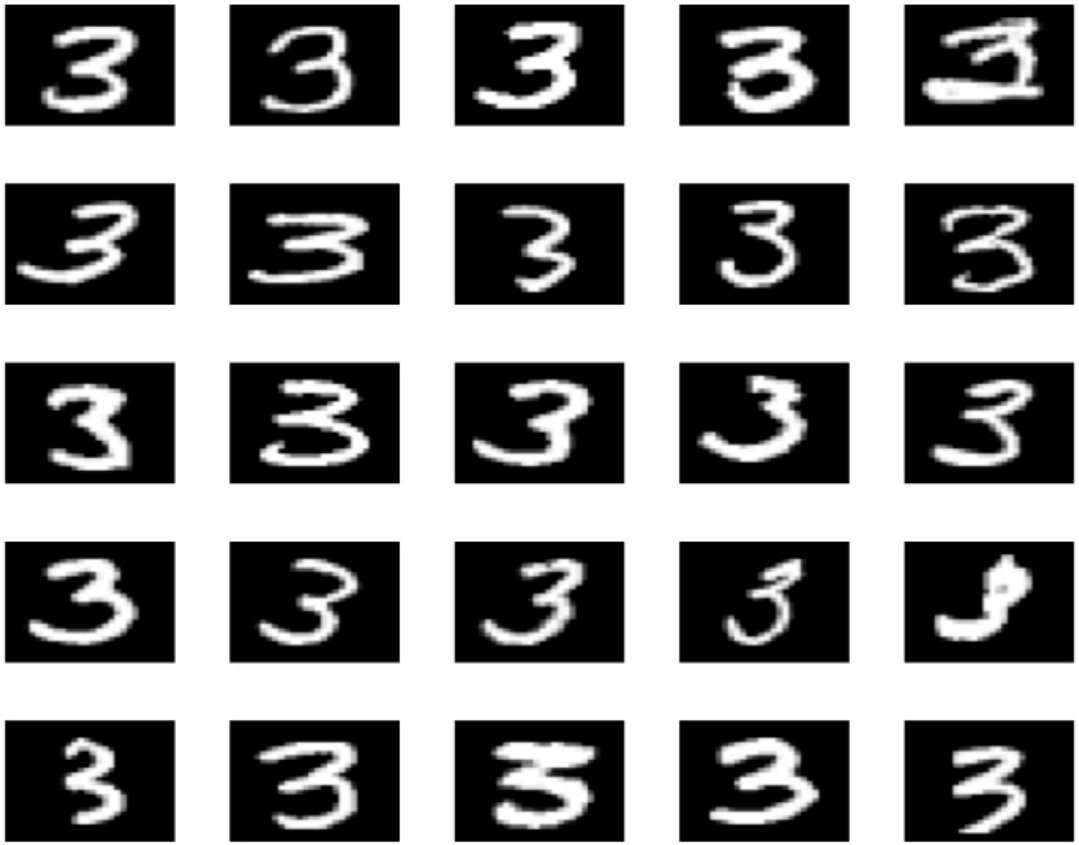
- Consider running PCA on 2429 19x19 grayscale images (CBCL data)
- Can get good reconstructions with only 3 components

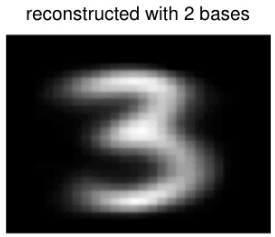
- PCA for pre-processing: can apply classifier to latent representation
  - Original data is 361 dimensional
  - For face recognition PCA with 3 components obtains 79% accuracy on face/non-face discrimination on test data vs. 76.8% for a Gaussian mixture model (GMM) with 84 states. (We'll cover GMMs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

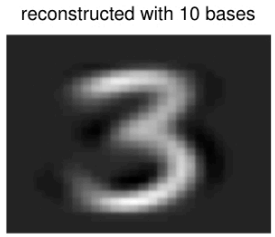
Applying PCA to faces: Learned basis

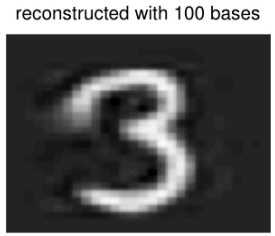
Principal components of face images ("eigenfaces")

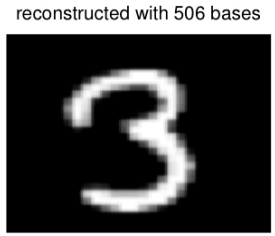
Applying PCA to digits

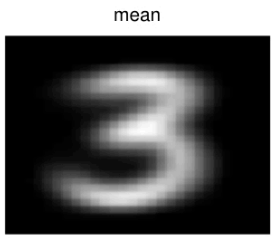


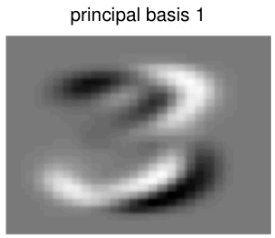


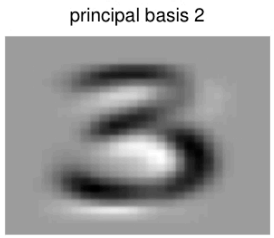


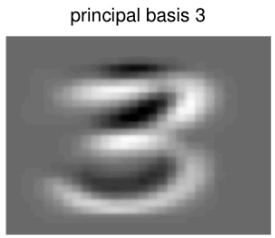










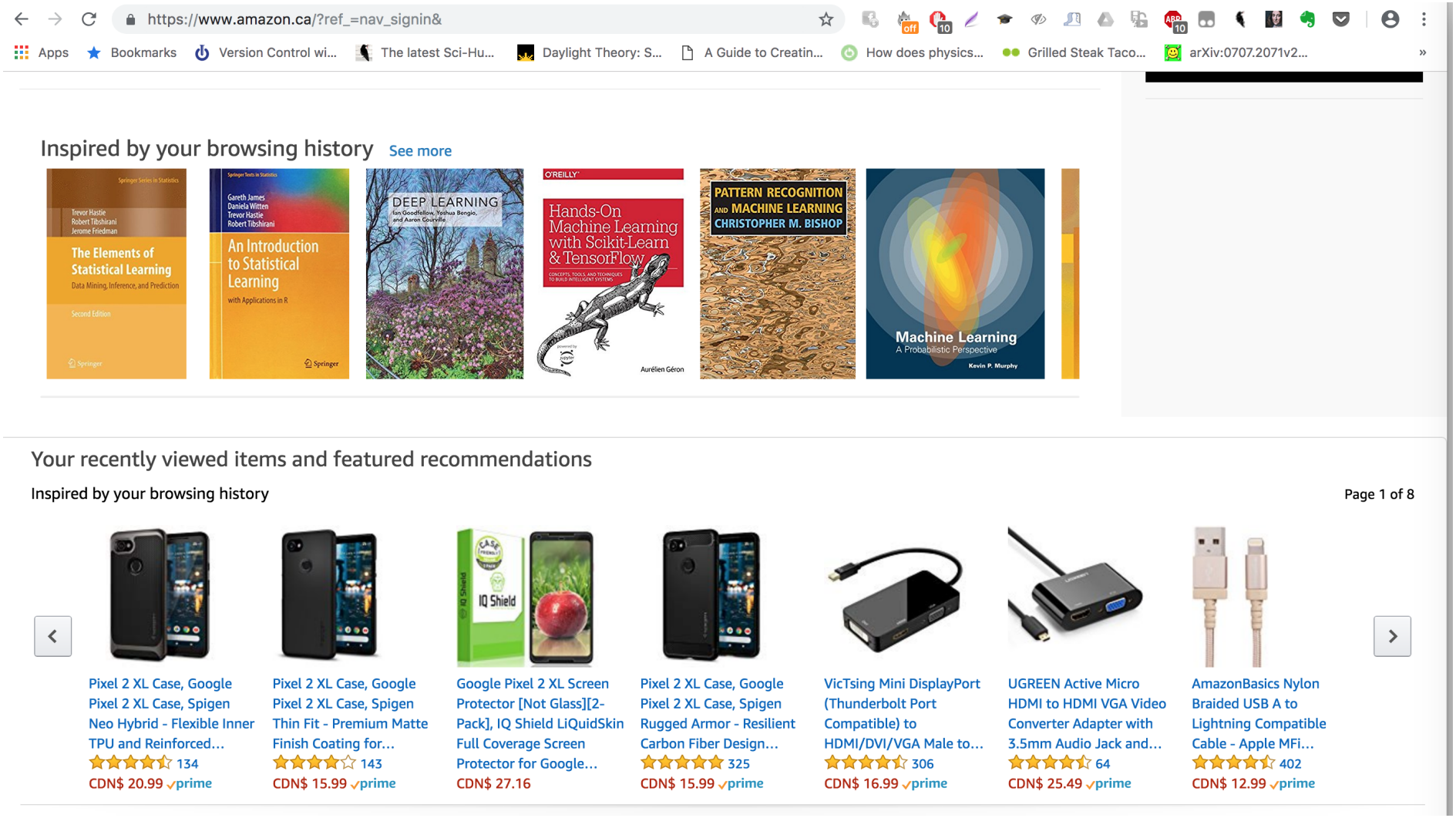


Next

Two more interpretations of PCA, which have interesting generalizations.

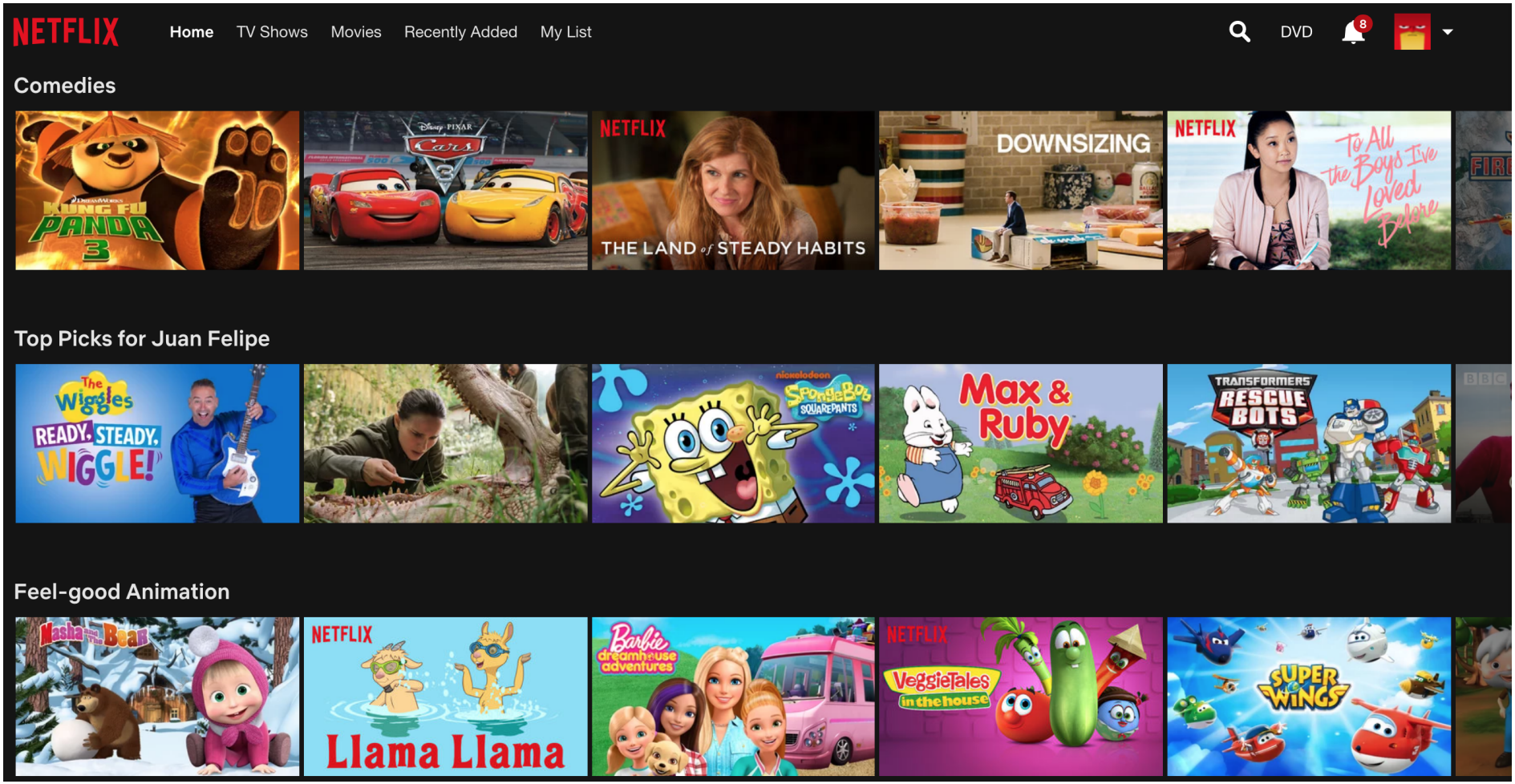
1. **Matrix factorization**
2. Autoencoder

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★.

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 a Matrix Factorization

- Recall PCA: project data onto a low-dimensional subspace defined by the top eigenvalues of the data covariance
- Today we consider a generalization, matrix factorizations
  - view PCA as a matrix factorization problem
  - extend to matrix completion, where the data matrix is only partially observed
  - extend to other matrix factorization models, which place different kinds of structure on the factors

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: $\hat{\boldsymbol{\mu}} = 0$. 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

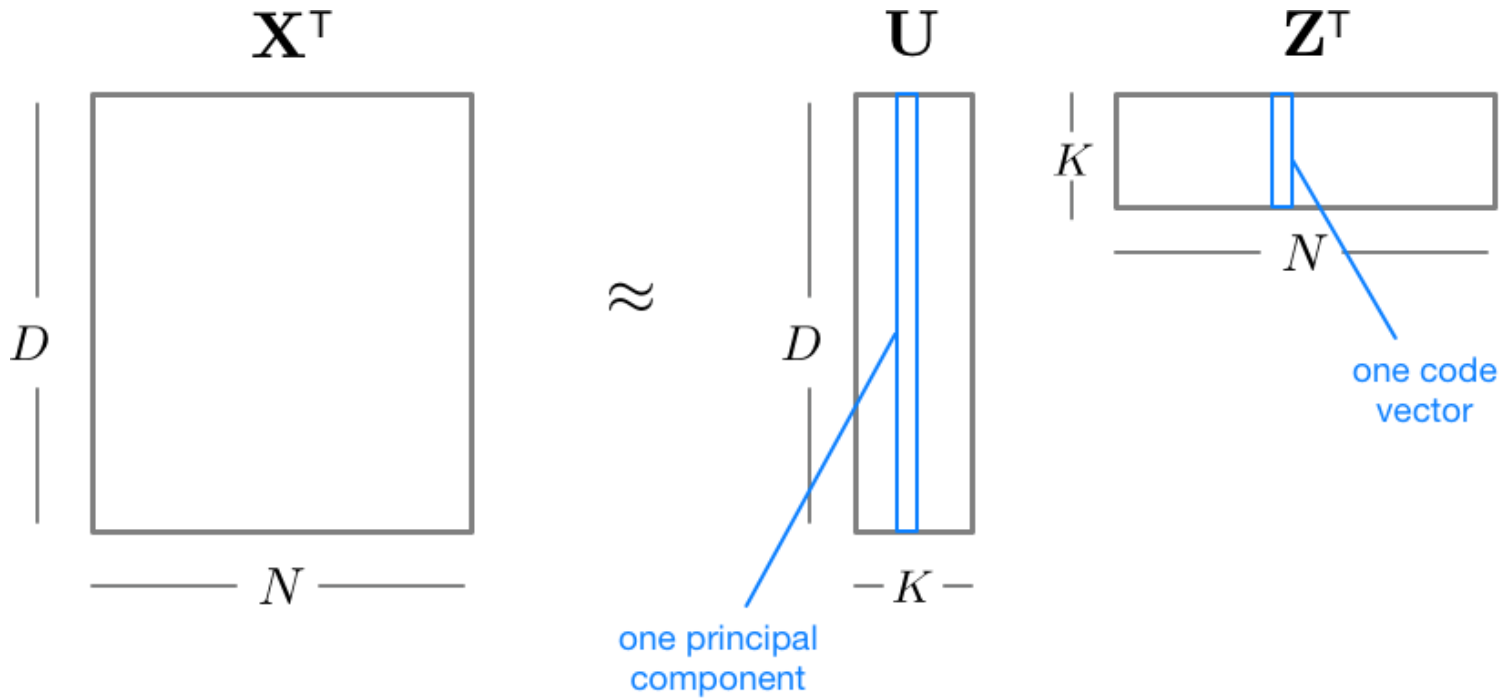
$$\sum_{i=1}^{N} \|\mathbf{x}^{(i)} - \mathbf{U}\mathbf{z}^{(i)}\|^2 = \|\mathbf{X} - \mathbf{Z}\mathbf{U}^\top\|_F^2,$$

- $\|\cdot\|_F$ 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 $\|\mathbf{X}^\top - \mathbf{U}\mathbf{Z}^\top\|_F^2$.

Supplement: Singular-Value Decomposition (SVD)

This has a close relationship to the Singular Value Decomposition (SVD) of $\mathbf{X}$ which is a matrix factorization technique. Consider an $N \times D$ matrix $\mathbf{X} \in \mathbb{R}^{N \times D}$ with SVD

$$\mathbf{X} = \mathbf{Q}\mathbf{S}\mathbf{U}^\top$$

Properties:

- $\mathbf{Q}$, $\mathbf{S}$, and $\mathbf{U}^\top$ provide a real-valued matrix factorization of $\mathbf{X}$.
- $\mathbf{Q}$ is a $N \times D$ matrix with orthonormal columns, $\mathbf{Q}^\top \mathbf{Q} = \mathbf{I}_D$, where $\mathbf{I}_D$ is the $D \times D$ identity matrix.
- $\mathbf{U}$ is an orthonormal $D \times D$ matrix, $\mathbf{U}^\top = \mathbf{U}^{-1}$.
- $\mathbf{S}$ is a $D \times D$ diagonal matrix, with non-negative singular values, $s_1, s_2, \ldots, s_D$, on the diagonal, where the singular values are conventionally ordered from largest to smallest.

Note that standard SVD notation is $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$. We are using $\mathbf{X} = \mathbf{Q}\mathbf{S}\mathbf{U}^\top$ for notational convenience.

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

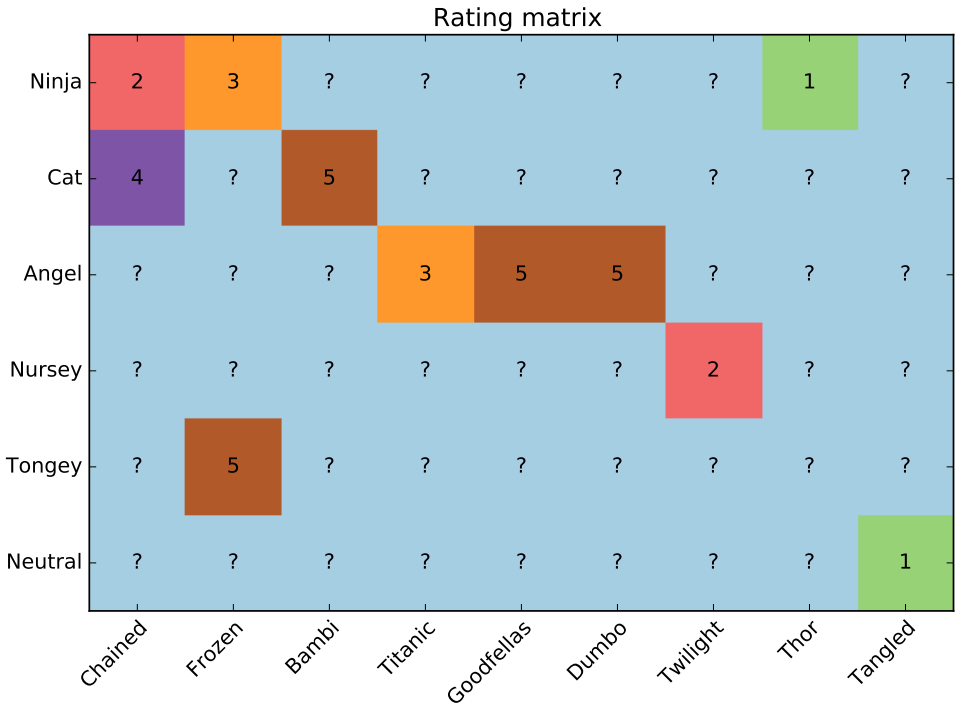
Movie recommendation: Users watch movies and rate them as good or bad.

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 $\mathbf{R}$



- **Data**: Users rate some movies. $\mathbf{R}_{\text{user,movie}}$. 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 $\mathbf{u}_i$ 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

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

  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

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

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

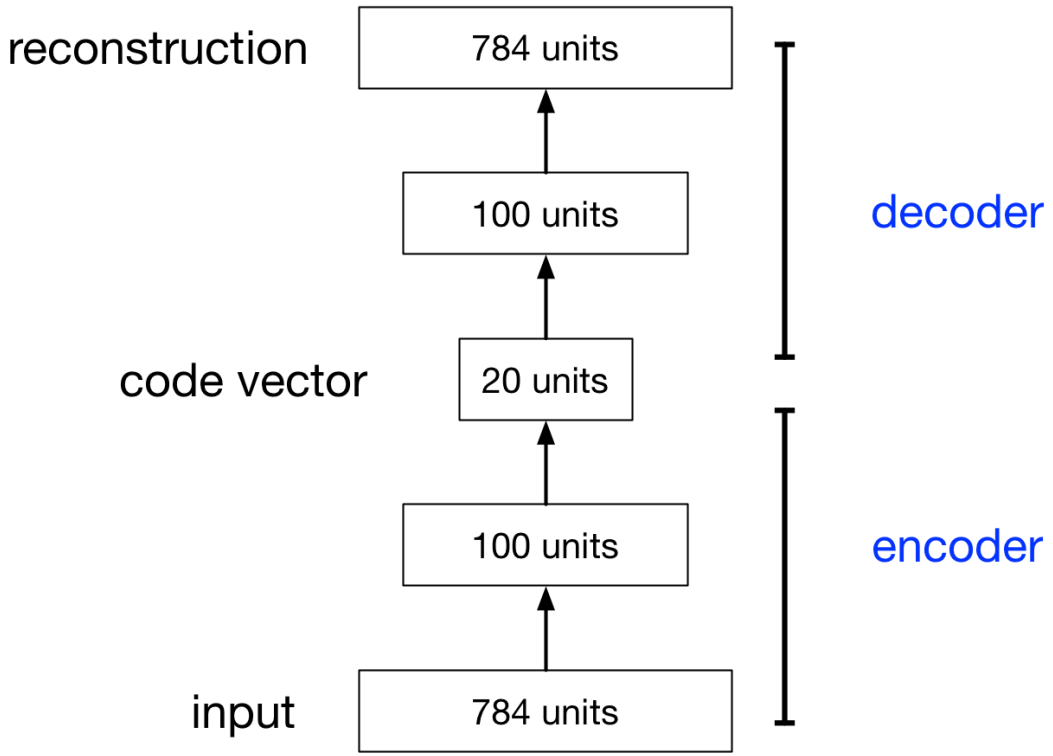
Next

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

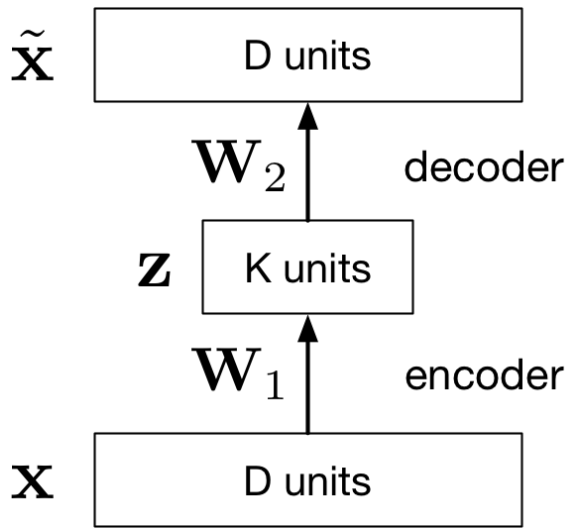
Why autoencoders?

- 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
  - Unlabled 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.

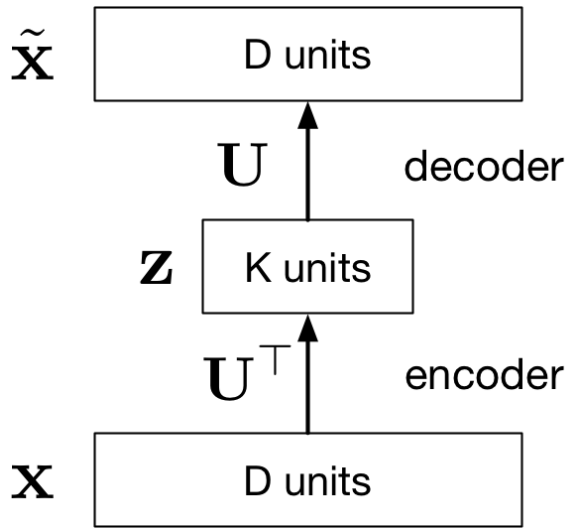
$$\mathcal{L}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|^2$$



- 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.

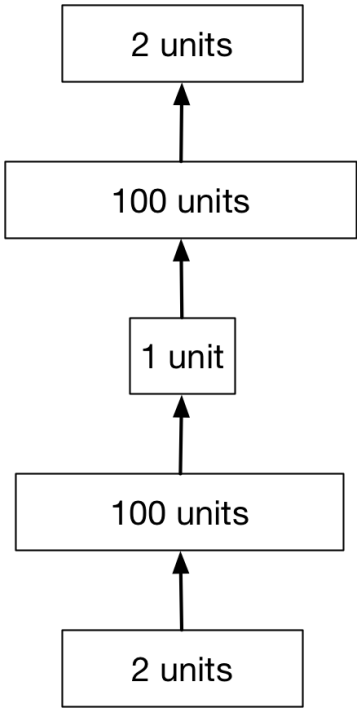
Linear Autoencoders

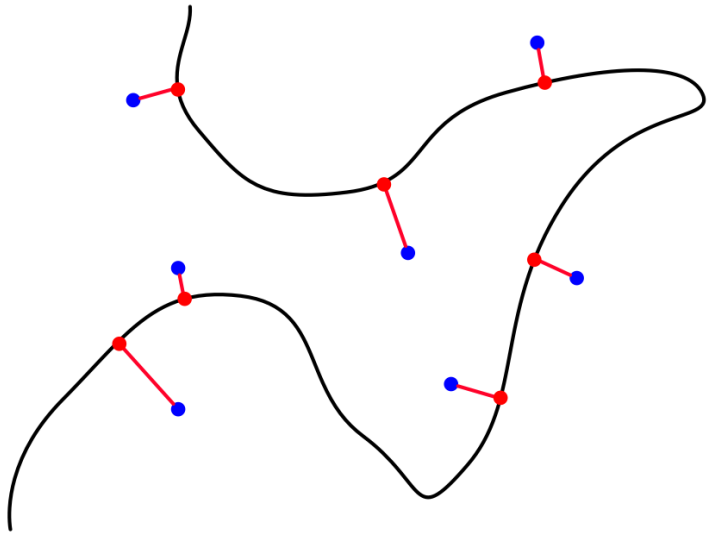
- Observe that the output of the autoencoder must lie in a K-dimensional subspace spanned by the columns of $\mathbf{W}_2$. This is because $\tilde{\mathbf{x}} = \mathbf{W}_2\mathbf{z}$
- We saw that the best possible (min error) K-dimensional linear subspace in terms of reconstruction error is the PCA 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

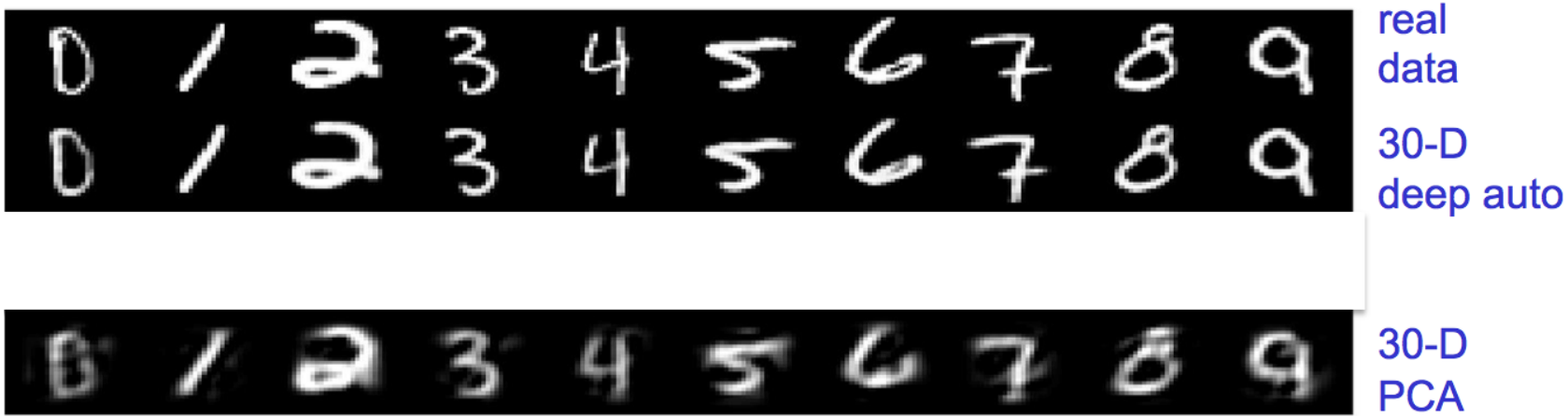
- Deep nonlinear autoencoders learn to project the data, not onto a subspace, but onto a nonlinear manifold
- This manifold is the image of the decoder.
- This is a kind of nonlinear dimensionality reduction.





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.