CSC 311: Introduction to Machine Learning

Lecture 8 - Principal Component Analysis

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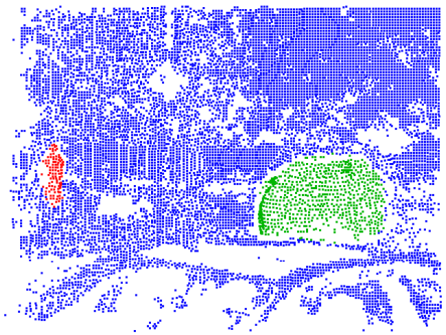
Unsupervised Learning: Motivating Examples

- Some examples of situations where you'd use unsupervised learning
  - You want to understand how a scientific field has changed over time. You want to take a large database of papers and model how the distribution of topics changes from year to year. But what are the topics?
  - You're a biologist studying animal behavior, so you want to infer a high-level description of their behavior from video. You don't know the set of behaviors ahead of time.
  - You want to reduce your energy consumption, so you take a time series of your energy consumption over time, and try to break it down into separate components (refrigerator, washing machine, etc.).
- Common theme: you have some data, and you want to infer the structure underlying the data.
- This structure is latent, which means it's never observed.

Motivating Examples

- Determine groups of people in image above
  - based on clothing styles
  - gender, age, etc

- Determine moving objects in videos

Overview

- Today we'll cover the first unsupervised learning algorithm for this course: principal component analysis (PCA)
- Dimensionality reduction: map the data to a lower dimensional space
  - Save computation/memory
  - Reduce overfitting, achieve better generalization
  - Visualize in 2 dimensions
- PCA is a linear model. It's useful for understanding lots of other algorithms.
  - Autoencoders
  - Matrix factorizations (in 2 weeks)
- Today's lecture is very linear-algebra-heavy.
  - Especially orthogonal matrices and eigendecompositions.
  - Don't worry if you don't get it immediately — next few lectures won't build on it. Tutorials 6&7 review some of the relevant topics.

Setup: Multivariate Parameters

- Set-up: given a iid dataset $\mathcal{D} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\} \subset \mathbb{R}^D$.
- N instances/observations/examples

$$\mathbf{X} = \begin{bmatrix} [\mathbf{x}^{(1)}]^\top \\ [\mathbf{x}^{(2)}]^\top \\ \vdots \\ [\mathbf{x}^{(N)}]^\top \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_D^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_D^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(N)} & x_2^{(N)} & \cdots & x_D^{(N)} \end{bmatrix}$$

- Mean

$$\mathbb{E}[\mathbf{x}^{(i)}] = \boldsymbol{\mu} = [\mu_1, \cdots, \mu_D]^T \in \mathbb{R}^D$$

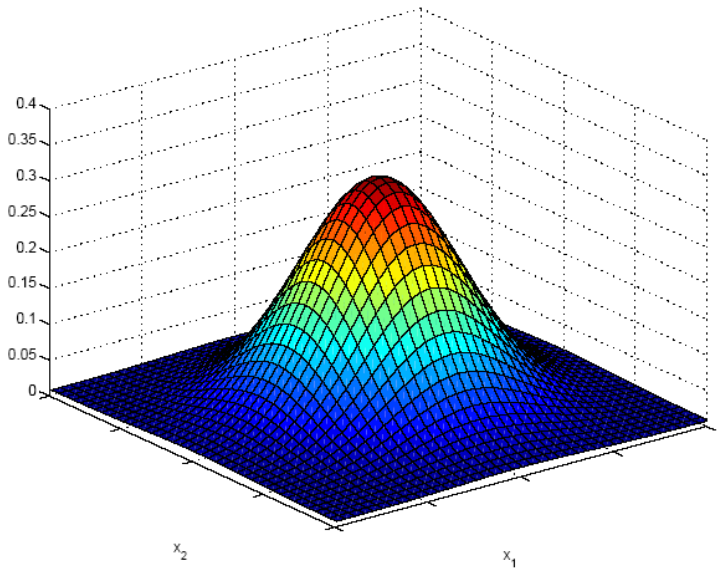
- Covariance

$$\boldsymbol{\Sigma} = Cov(\mathbf{x}^{(i)}) = \mathbb{E}[(\mathbf{x}^{(i)} - \boldsymbol{\mu})(\mathbf{x}^{(i)} - \boldsymbol{\mu})^\top] = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1D} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{D1} & \sigma_{D2} & \cdots & \sigma_D^2 \end{bmatrix}$$

Multivariate Gaussian Model

- $\mathbf{x}^{(i)} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, a Gaussian (or normal) distribution defined as

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$



Mean and Covariance Estimators

- Observe data $\mathcal{D} = \{\mathbf{x}^{(1)}, ..., \mathbf{x}^{(N)}\}$.
- Recall that the MLE estimators for the mean $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ under the multivariate Gaussian model is given by (previous lecture)

$$\text{Sample mean:} \quad \hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}^{(i)}$$

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

- Roughly, $\hat{\boldsymbol{\mu}}$ quantifies where your data is located in space.
- $\hat{\boldsymbol{\Sigma}}$ quantifies the shape of spread of your data points.

Bivariate Normal

$$\boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$$

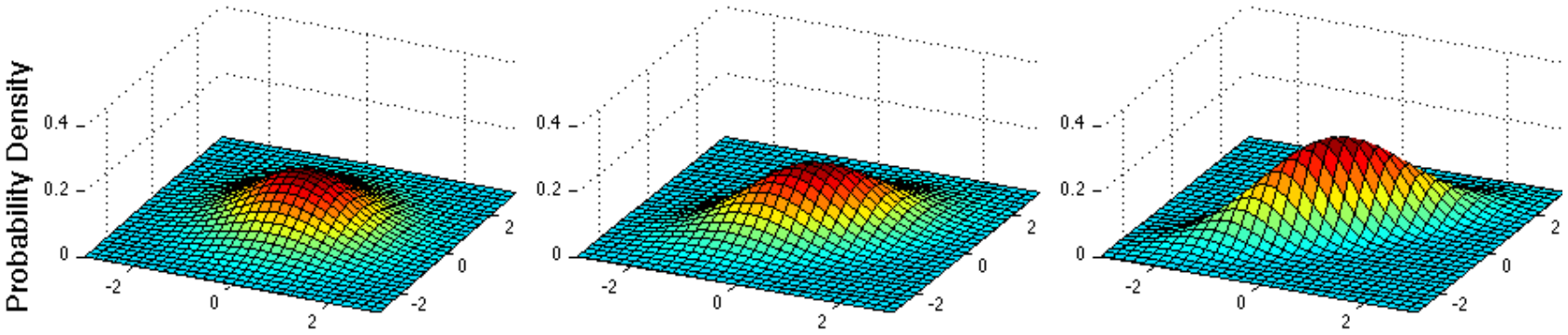


Figure: Probability density function

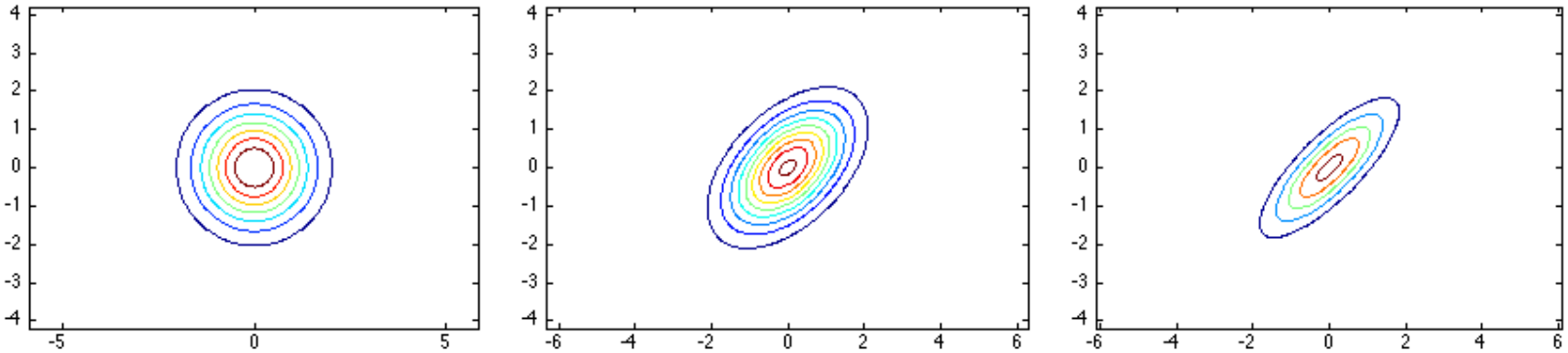
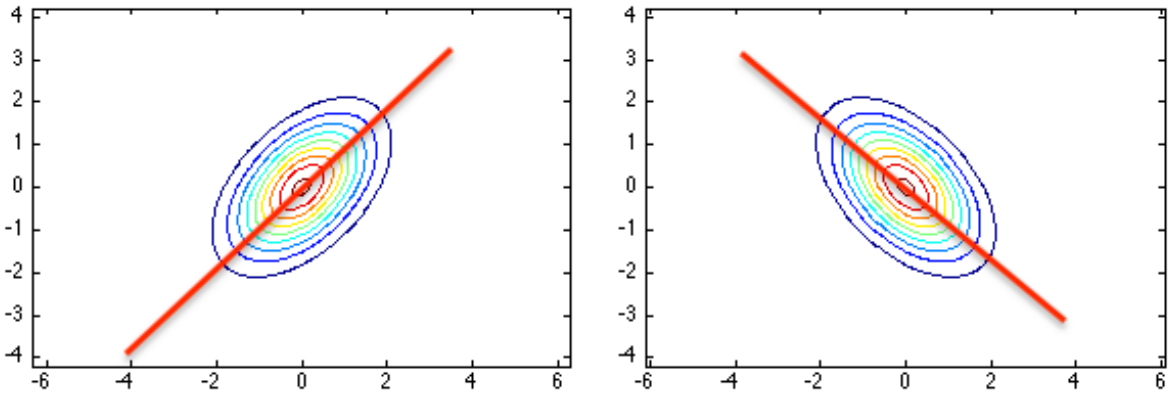


Figure: Contour plot of the pdf

Low dimensional representation

- In practice, even though data is very high dimensional, its important features can be accurately captured in a low dimensional subspace.



- Find a low dimensional representation of your data.
  - Computational benefits
  - Interpretability, visualization
  - Generalization

Low dimensional representation

- In practice, even though data is very high dimensional, its important features can be accurately captured in a low dimensional subspace.

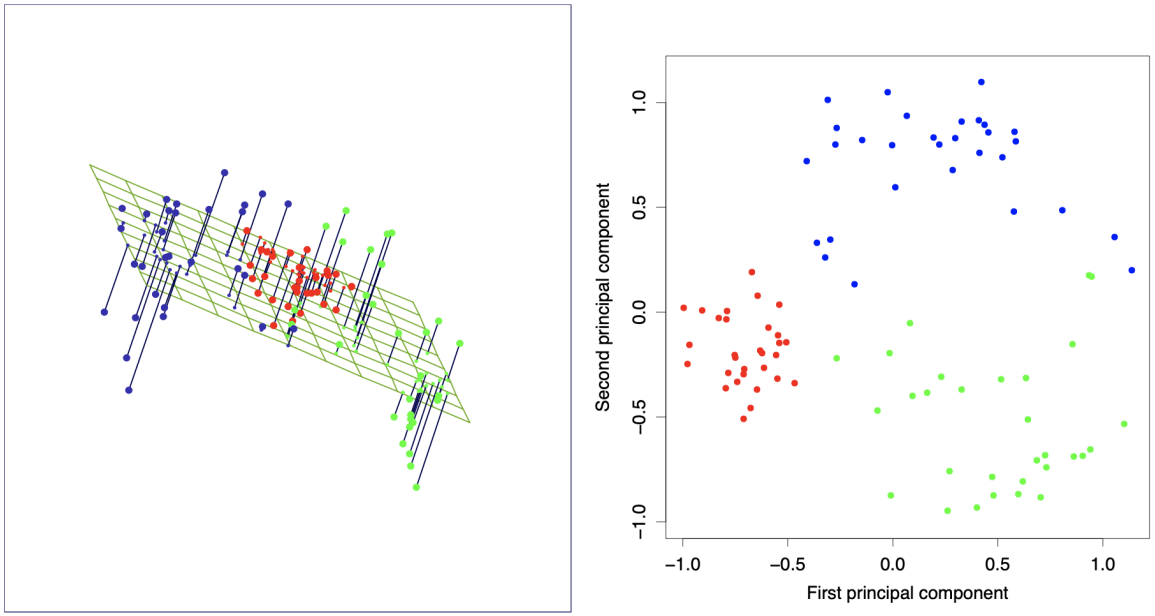
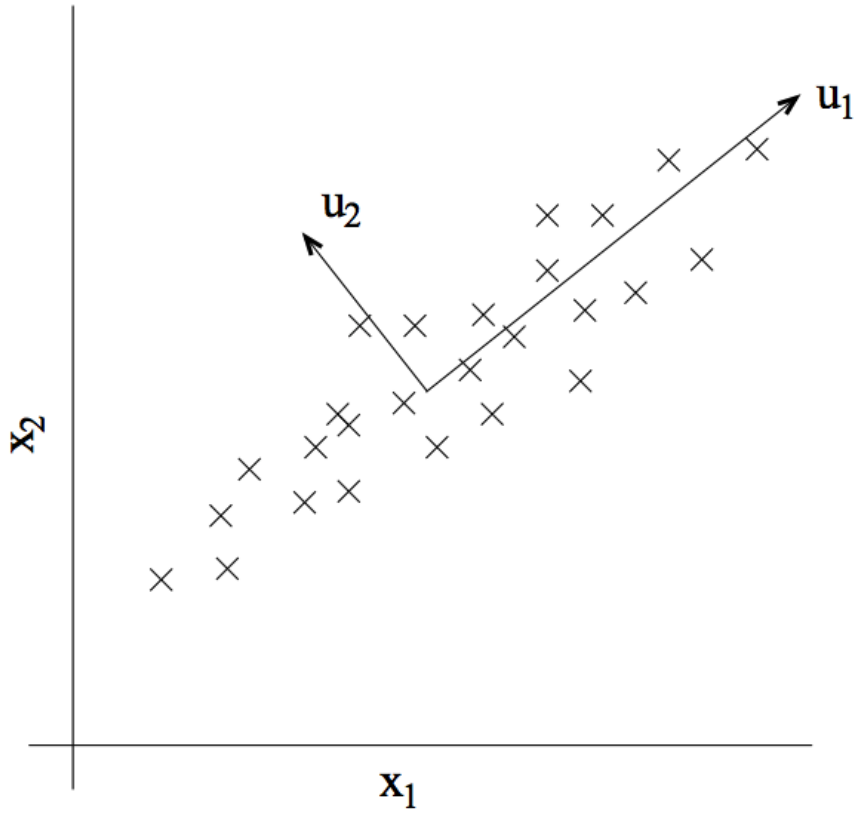


Image credit: Elements of Statistical Learning

Projection onto a subspace

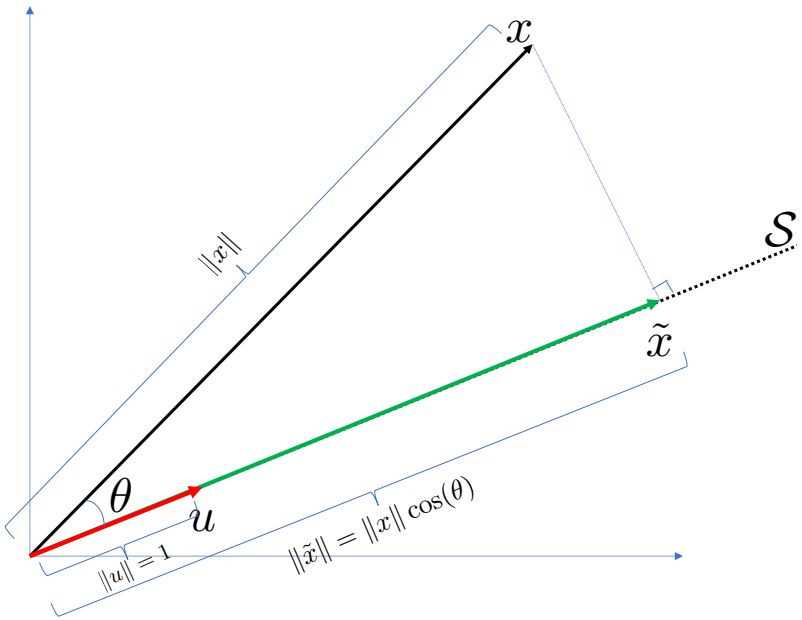
- Set-up: given a dataset $\mathcal{D} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\} \subset \mathbb{R}^D$
- Set $\hat{\boldsymbol{\mu}}$ to the sample mean of the data, $\hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}^{(i)}$
- Goal: find a K-dimensional subspace $\mathcal{S} \subset \mathbb{R}^D$ such that $\mathbf{x}^{(n)} - \hat{\boldsymbol{\mu}}$ is "well-represented" by its projection onto a K-dimensional $\mathcal{S}$
- Recall: The projection of a point $\mathbf{x}$ onto $\mathcal{S}$ is the point in $\mathcal{S}$ closest to $\mathbf{x}$. More on this coming soon.

We are looking for directions



- For example, in a 2-dimensional problem, we are looking for the direction $\boldsymbol{u}_1$ along which the data is well represented: (?)
  - e.g. direction of higher variance
  - e.g. direction of minimum difference after projection
  - turns out they are the same!

Euclidean projection



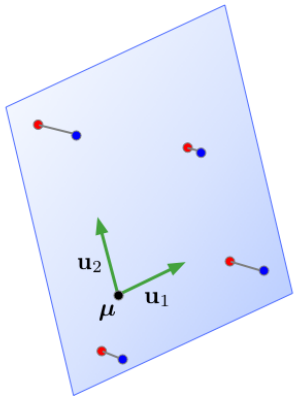
- Here, $\mathcal{S}$ is the line along the unit vector $\mathbf{u}$ (1-dimensional subspace)
  - $\mathbf{u}$ is a basis for $\mathcal{S}$: any point in $\mathcal{S}$ can be written as $z\mathbf{u}$ for some z.

- 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

- In general, $\mathcal{S}$ is not one dimensional (i.e. line), but a subspace with higher dimension K.

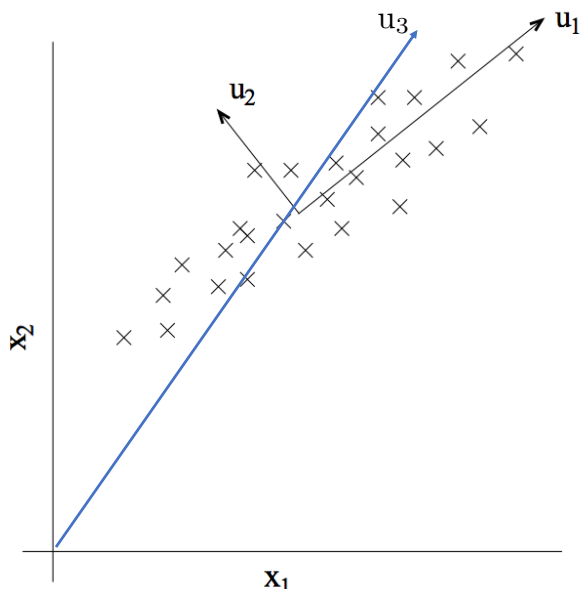
- In this case, we have K basis vectors $\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_K \in \mathbb{R}^D$: any vector $\mathbf{y}$ in $\mathcal{S}$ can be written as $\mathbf{y} = \sum_{i=1}^{K} z_i \mathbf{u}_i$ for some $z_1 \cdots z_K$.

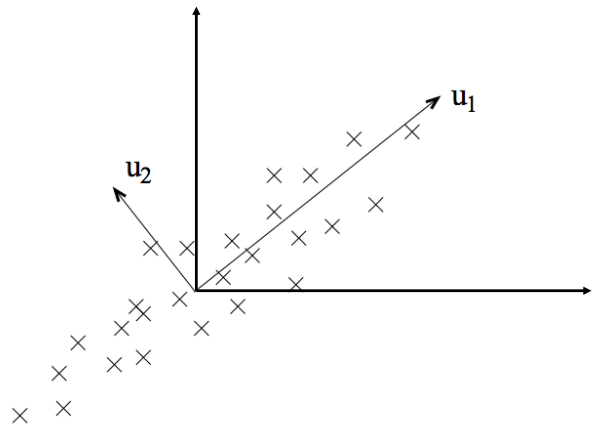


- Projection of $\mathbf{x}$ on this subspace is given as

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

First step: Center data





- Directions we compute will pass through origin, and should represent the direction of highest variance.
- We need to center our data since we don't want location of data to influence our calculations. We are only interested in finding the direction of highest variance. This is independent from its mean.
- $\Longrightarrow$ We are **not** interested in u_3, we are interested in u_1.

Projection onto a subspace

- Let $\{\mathbf{u}_k\}_{k=1}^K$ be an orthonormal basis of the subspace $\mathcal{S}$
- Approximate each data point $\mathbf{x}$ as:
  1. Center (subtract the mean)
  2. Project on $\mathcal{S}$
  3. Add the mean back

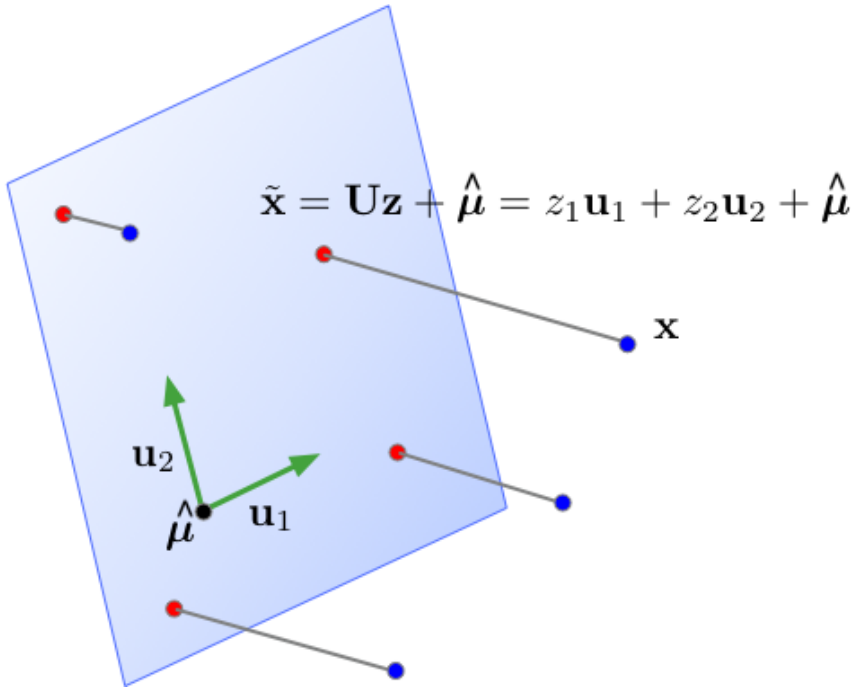
$$\begin{aligned}\tilde{\mathbf{x}} &= \hat{\boldsymbol{\mu}} + \text{Proj}_{\mathcal{S}}(\mathbf{x} - \hat{\boldsymbol{\mu}}) \\ &= \hat{\boldsymbol{\mu}} + \sum_{k=1}^{K} z_k \mathbf{u}_k\end{aligned}$$

- We also know: $z_k = \mathbf{u}_k^T(\mathbf{x} - \hat{\boldsymbol{\mu}})$
- Let $\mathbf{U}$ be a matrix with columns $\{\mathbf{u}_k\}_{k=1}^K$ then $\mathbf{z} = \mathbf{U}^T(\mathbf{x} - \hat{\boldsymbol{\mu}})$
- Also: $\tilde{\mathbf{x}} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{z} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{U}^T(\mathbf{x} - \hat{\boldsymbol{\mu}})$
- Here, $\mathbf{U}\mathbf{U}^T$ is the projector on $\mathcal{S}$, and $\mathbf{U}^T\mathbf{U} = I$

Projection on subspace

- Note that $\mathbf{x}$ and $\tilde{\mathbf{x}}$ have the same dimensionality. That is, they are both in $\mathbb{R}^D$.
- But $\tilde{\mathbf{x}}$ lives in a low dimensional subspace in $\mathbb{R}^D$.
- Its low dimensional representation is $\mathbf{z} \in \mathbb{R}^K$.

Projection onto a Subspace

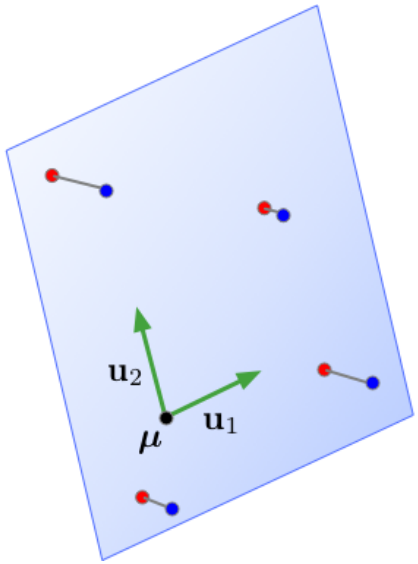


$$\mathbf{z} = \mathbf{U}^\top(\mathbf{x} - \hat{\boldsymbol{\mu}})$$

- 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 dimension reduction.



Learning a Subspace

- How to choose a good subspace $\mathcal{S}$?
  - Need to choose $D \times K$ matrix $\mathbf{U}$ with orthonormal columns.
- Two criteria:
  - Minimize the reconstruction error: Find vectors in a subspace that are closest to data points.

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

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

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

  - The data and its reconstruction has 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**: $\|\mathbf{v}\|^2 = \mathbf{v}^\top\mathbf{v}$ and $\mathbf{U}^\top\mathbf{U} = I$; we have $\|\mathbf{U}\mathbf{v}\|^2 = \mathbf{v}^\top\mathbf{U}^\top\mathbf{U}\mathbf{v} = \|v\|^2$. Therefore,

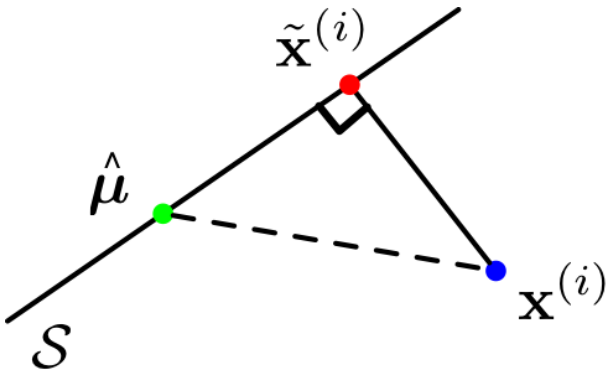
$$\|\tilde{\mathbf{x}}^{(i)}-\hat{\boldsymbol{\mu}}\|^2 = (\mathbf{U}\mathbf{z}^{(i)})^\top(\mathbf{U}\mathbf{z}^{(i)}) = [\mathbf{z}^{(i)}]^\top\mathbf{U}^\top\mathbf{U}\mathbf{z}^{(i)} = [\mathbf{z}^{(i)}]^\top\mathbf{z}^{(i)} = \|\mathbf{z}^{(i)}\|^2$$

Norm of centered reconstruction is equal to norm of representation.

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 $\frac{1}{N}\sum_i \mathbf{z}^{(i)} = 0$)

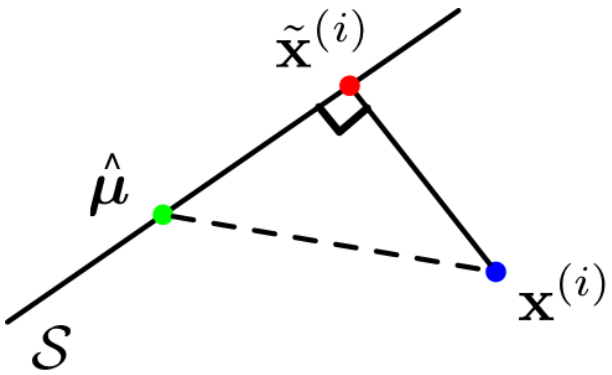
- **Observation 2**: orthogonality of $\tilde{\mathbf{x}}^{(i)} - \hat{\boldsymbol{\mu}}$ and $\tilde{\mathbf{x}}^{(i)} - \mathbf{x}^{(i)}$
  (Two vectors $\mathbf{a}, \mathbf{b}$ are orthogonal $\iff \mathbf{a}^\top \mathbf{b} = 0$)
- Recall $\tilde{\mathbf{x}}^{(i)} = \hat{\boldsymbol{\mu}} + \mathbf{U}\mathbf{U}^\top(\mathbf{x}^{(i)}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



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

Pythagorean Theorem

By averaging over data and from observation 2, we obtain



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

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

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

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).

Recall:

- Spectral Decomposition: a symmetric matrix $\mathbf{A}$ has a full set of eigenvectors, which can be chosen to be orthogonal. This gives a decomposition

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^\top,$$

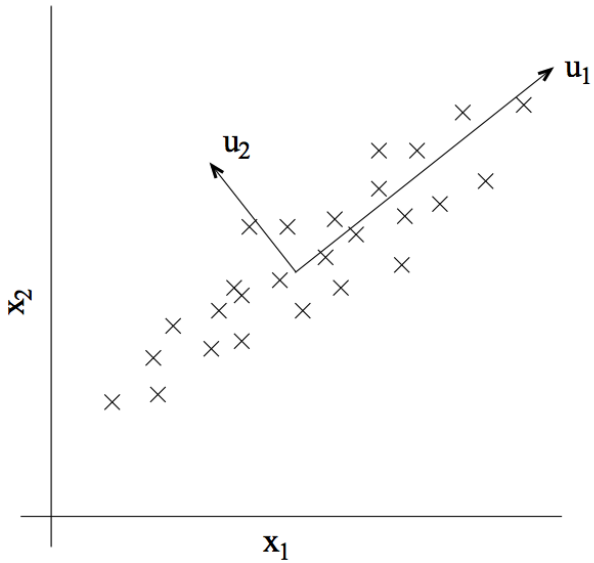
  where $\mathbf{Q}$ is orthogonal and $\mathbf{\Lambda}$ is diagonal. The columns of $\mathbf{Q}$ are eigenvectors, and the diagonal entries λ_j of $\mathbf{\Lambda}$ are the corresponding eigenvalues.
- I.e., symmetric matrices are diagonal in some basis.
- A symmetric matrix $\mathbf{A}$ is positive semidefinite iff each $\lambda_j \geq 0$.

Principal Component Analysis

- 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: Covariance matrices are 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.



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

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

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

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

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

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

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

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

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 $\mathbf{\Sigma}$. If you're interested, look up the Courant-Fischer Theorem.

Decorrelation

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

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

- 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

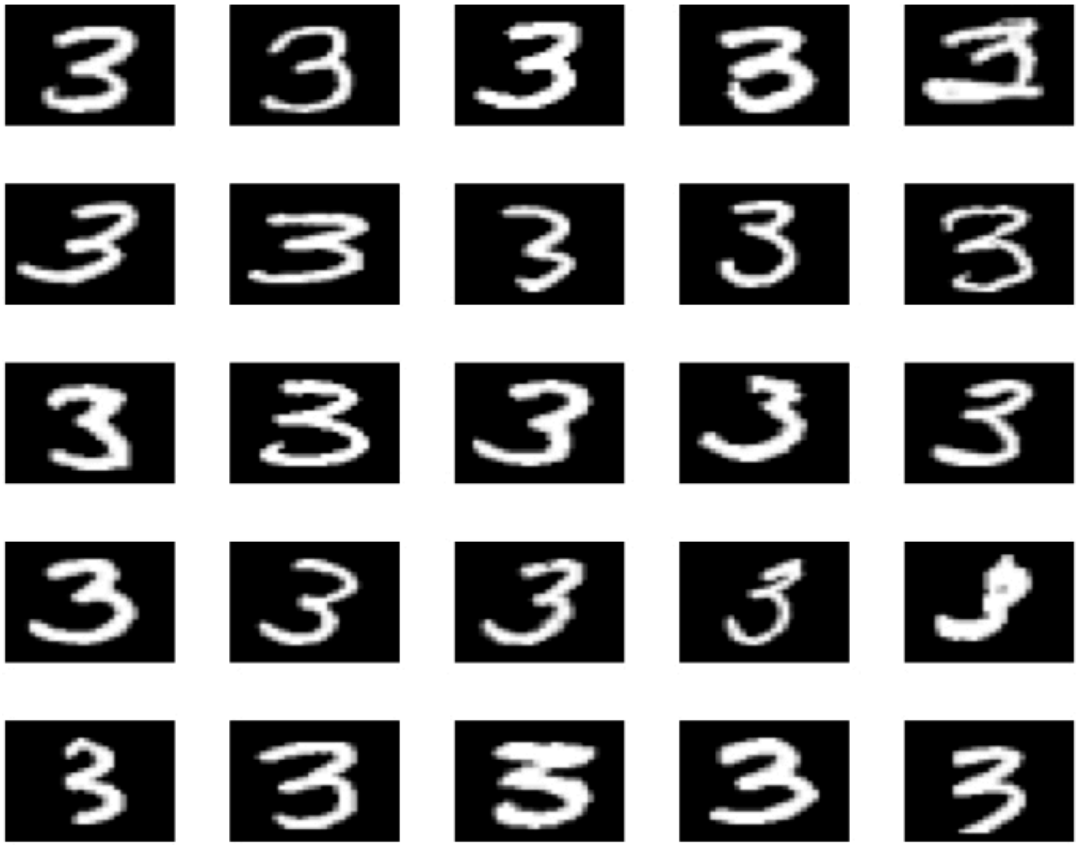
- Consider running PCA on 2429 19x19 grayscale images (CBCL data)
- Can get good reconstructions with only 3 components

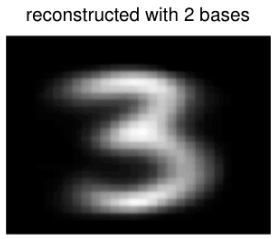
- PCA for pre-processing: can apply classifier to latent representation
  - Original data is 361 dimensional
  - For face recognition PCA with 3 components obtains 79% accuracy on face/non-face discrimination on test data vs. 76.8% for a Gaussian mixture model (GMM) with 84 states. (We'll cover GMMs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

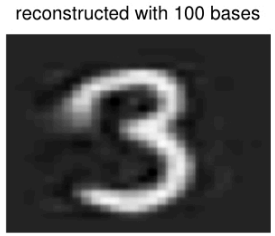
Applying PCA to faces: Learned basis

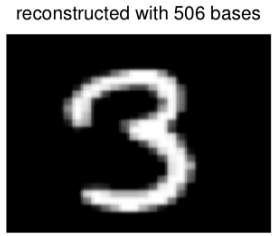
Principal components of face images ("eigenfaces")

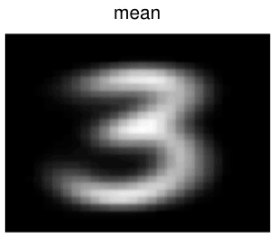
Applying PCA to digits

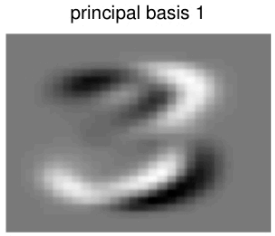


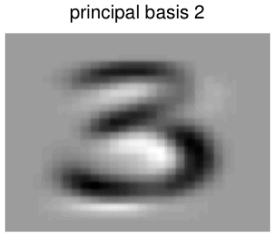


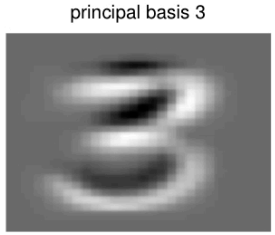












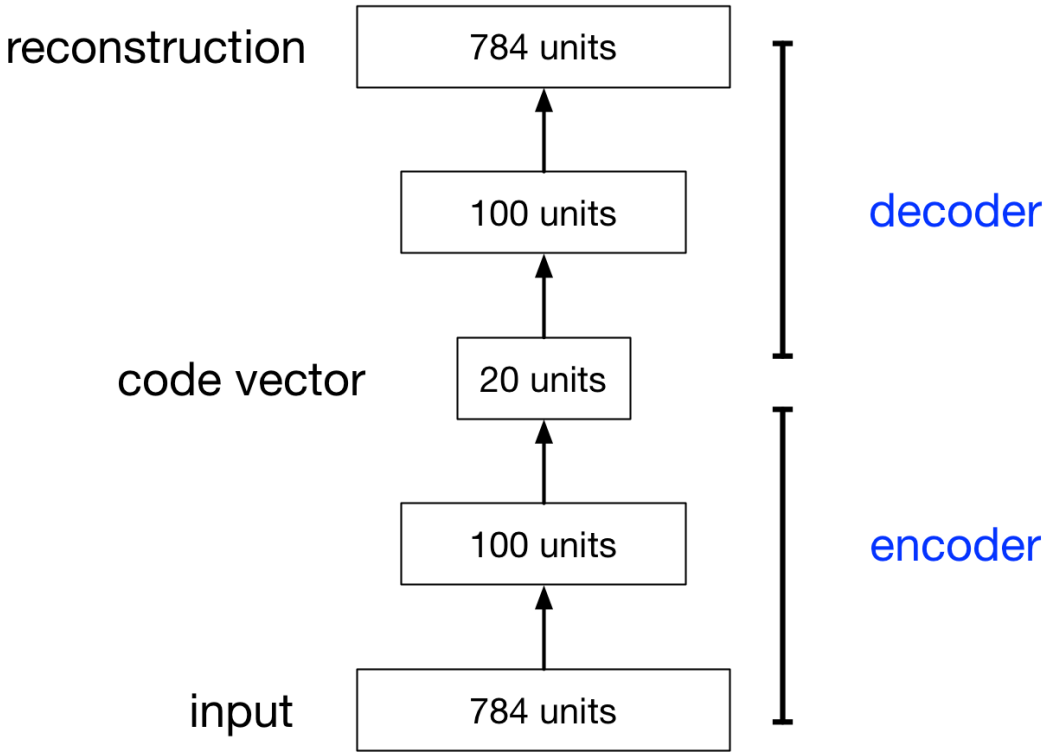
Next

Next: two more interpretations of PCA, which have interesting generalizations.

1. Autoencoders
2. Matrix factorization (later lecture)

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

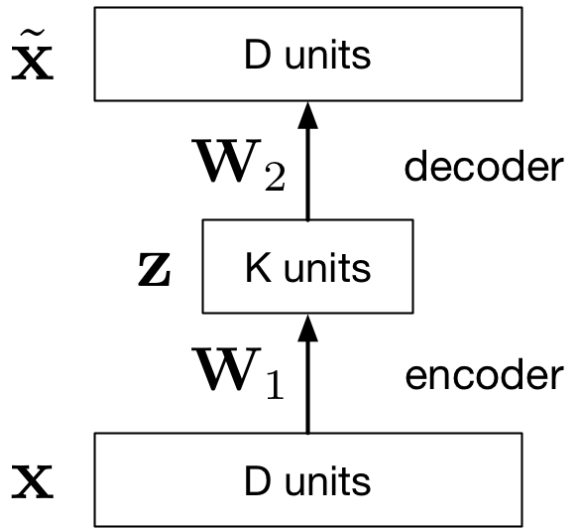
Why autoencoders?

- 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.

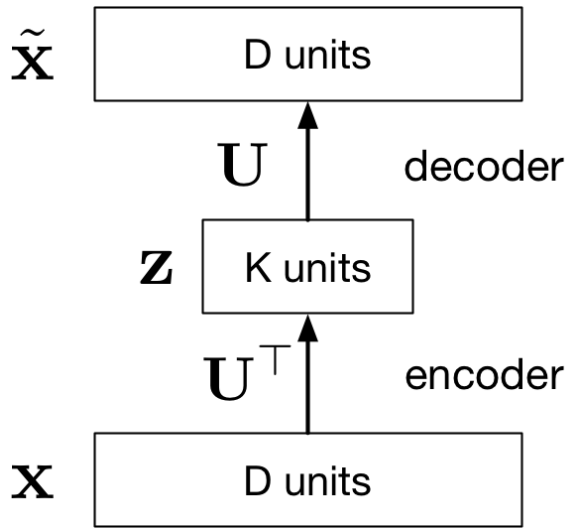
$$\mathcal{L}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|^2$$



- 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.

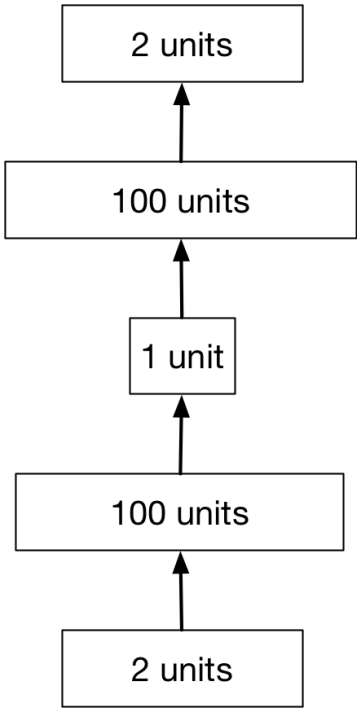
Linear Autoencoders

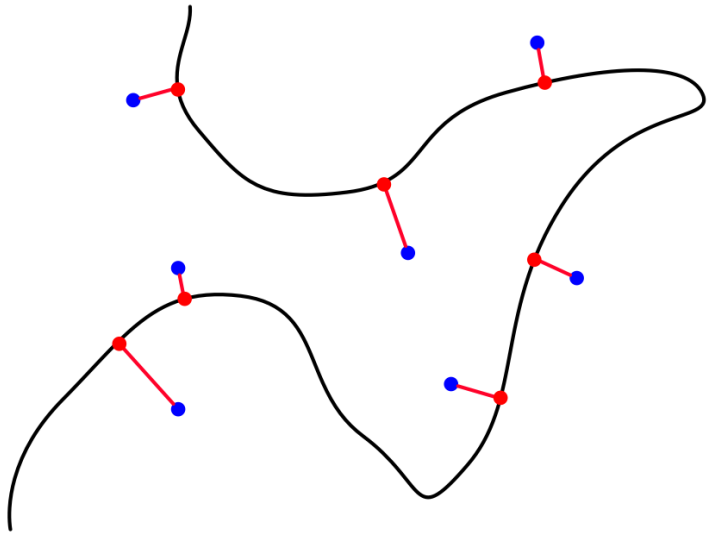
- Observe that the output of the autoencoder must lie in a K-dimensional subspace spanned by the columns of $\mathbf{W}_2$. This is because $\tilde{\mathbf{x}} = \mathbf{W}_2\mathbf{z}$
- We saw that the best possible (min error) K-dimensional linear subspace in terms of reconstruction error is the PCA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

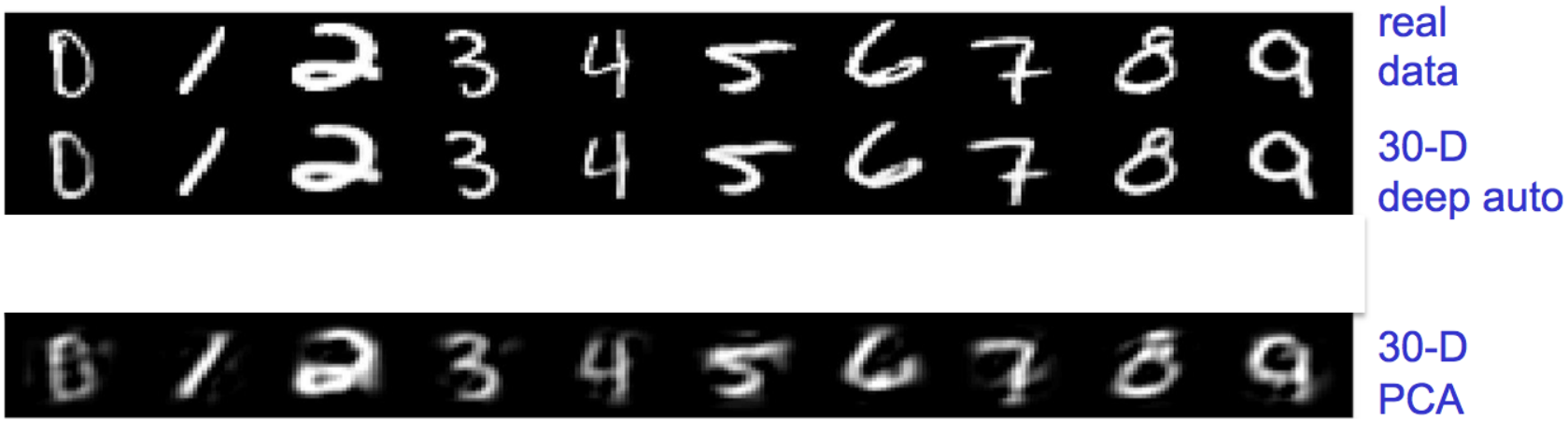
- Deep nonlinear autoencoders learn to project the data, not onto a subspace, but onto a nonlinear manifold
- This manifold is the image of the decoder.
- This is a kind of nonlinear dimensionality reduction.





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.