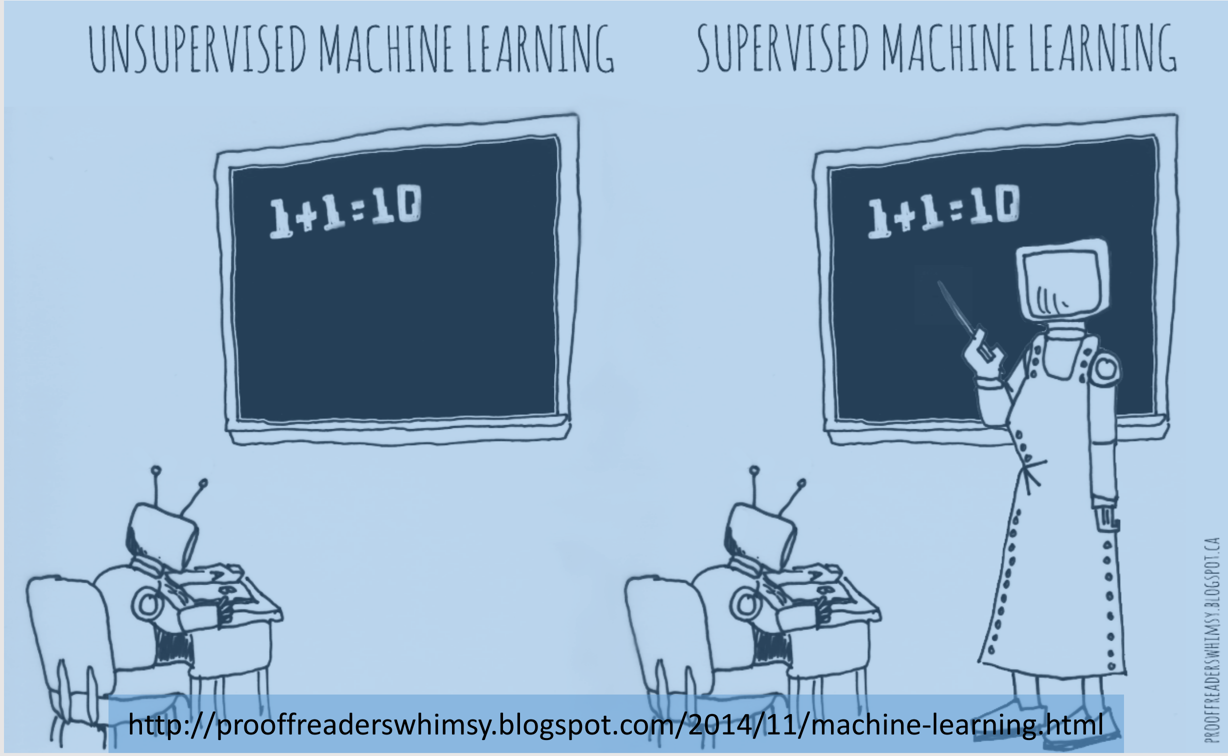
Lecture 8: Unsupervised Learning



[Haiping Lu](#)

YouTube Playlist: https://www.youtube.com/c/HaipingLu/playlists

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Week 8 Contents / Objectives

- Why Unsupervised Learning?
- Principal Component Analysis (PCA)
- PCA Unboxing
- Clustering: from k-means to spectral
- Autoencoder

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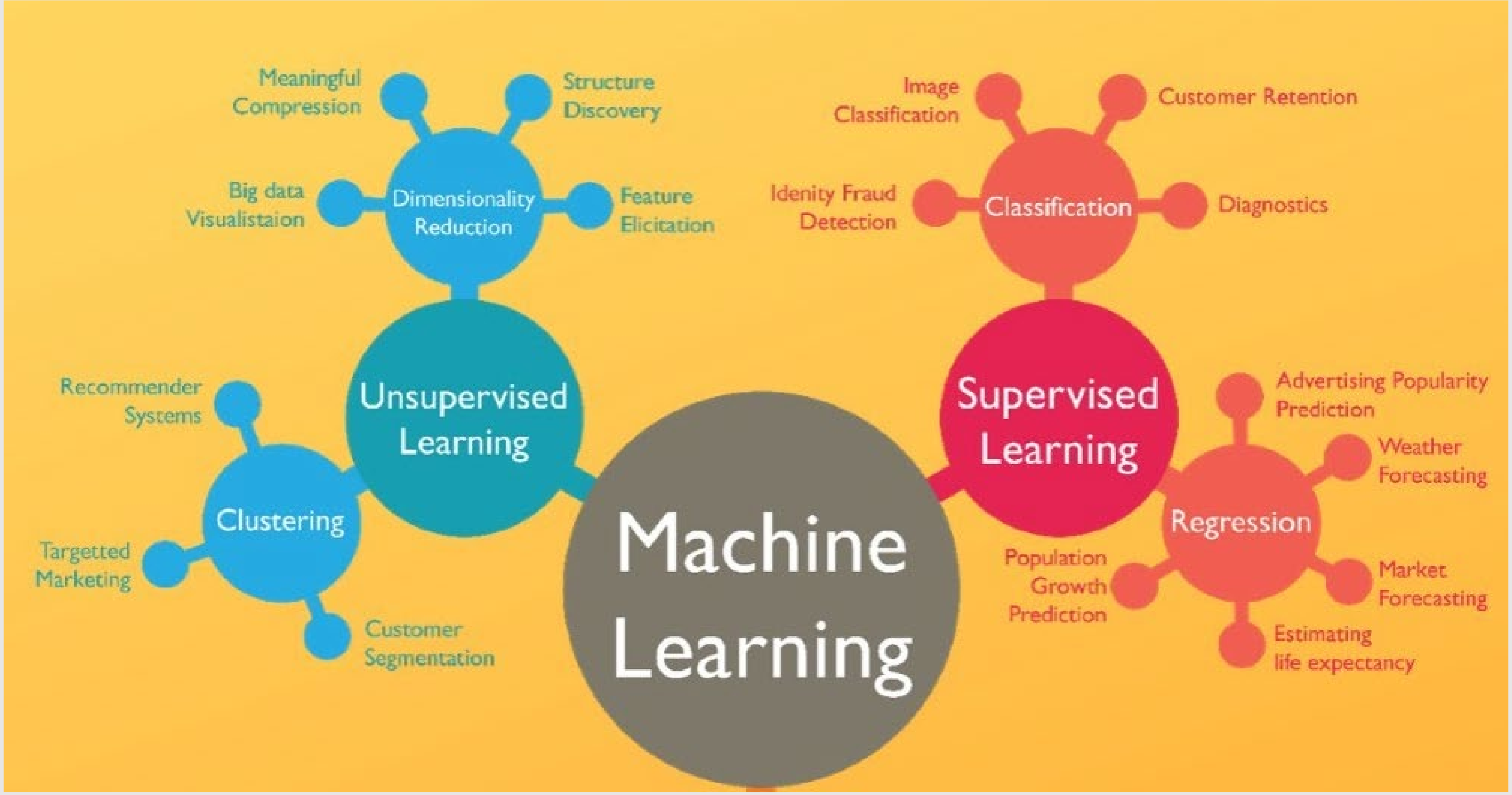
Supervised vs Unsupervised



https://i.morioh.com/2020/04/14/ff897f322fed.jpg

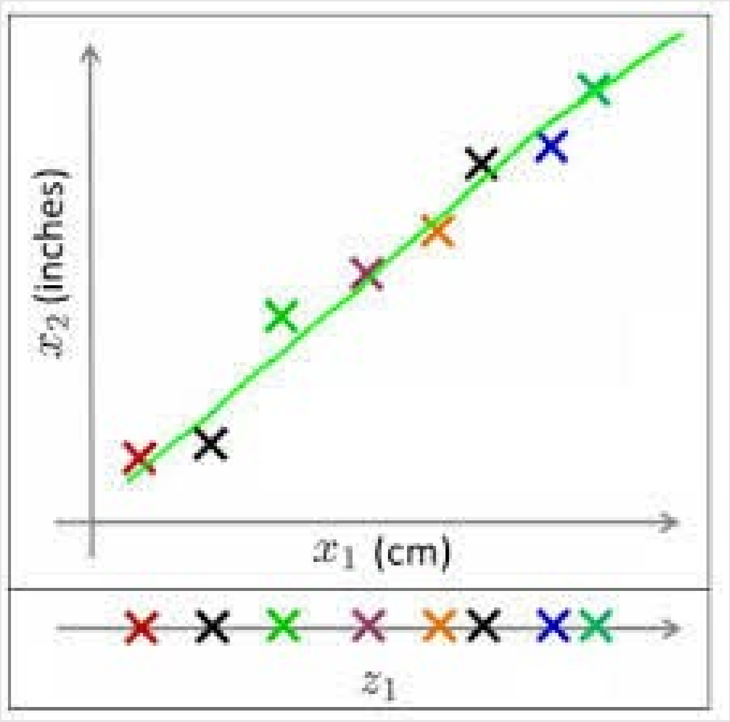
Unsupervised Learning

- Supervised learning: each data point has a label
- Unsupervised learning: no labels for the data
  - Dimensionality reduction
  - Clustering

Machine Learning	**Supervised**	**Unsupervised**
Discrete output	Classification	Clustering
Continuous output	Regression	Dimensionality Reduction

Dimensionality Reduction (DR)

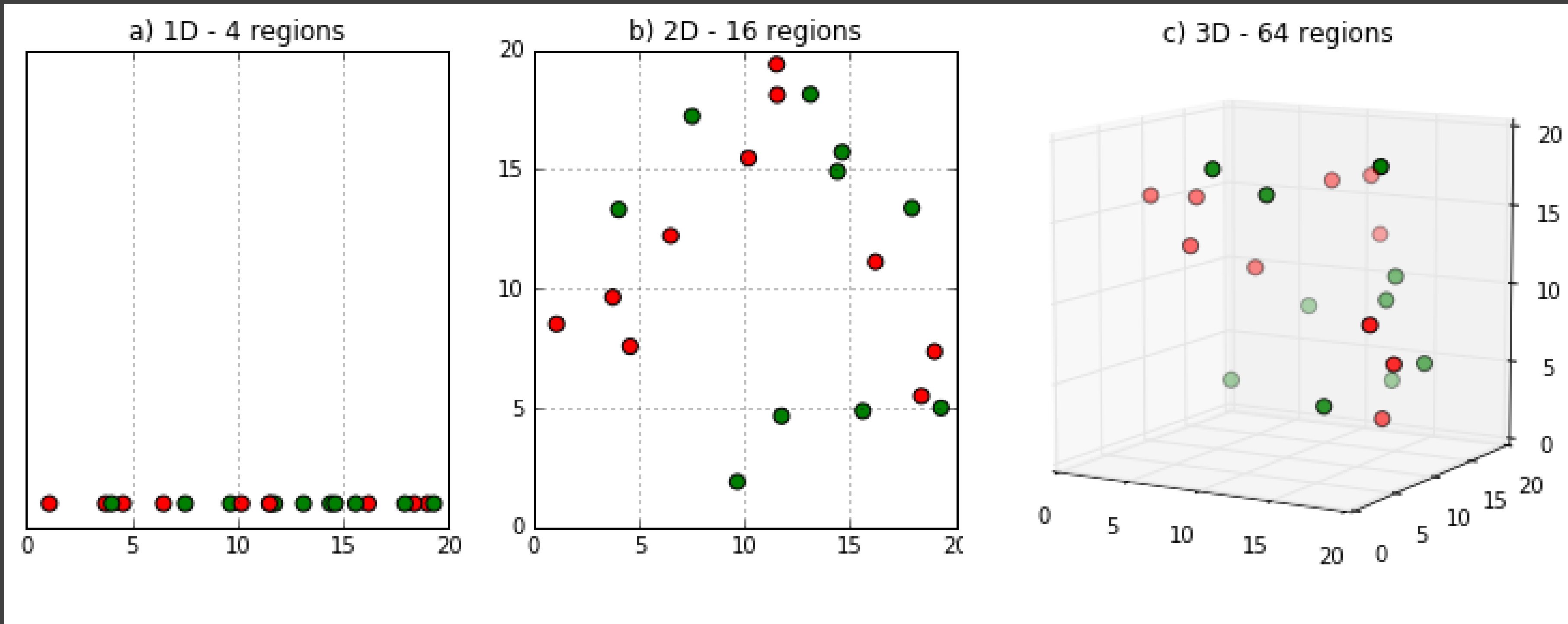
- 2 → 1



High Dimensional → Original data

Low Dimensional → Transformed

Original data	Transformed
(1, 1.2)	1.15
(2, 2)	2
(3, 3.3)	3.1
…	…



Why DR?
High D → Low D

- **Curse of dimensionality**
  - **Nearest neighbours**
- Reduce redundancy (correlation)
- Visualisation

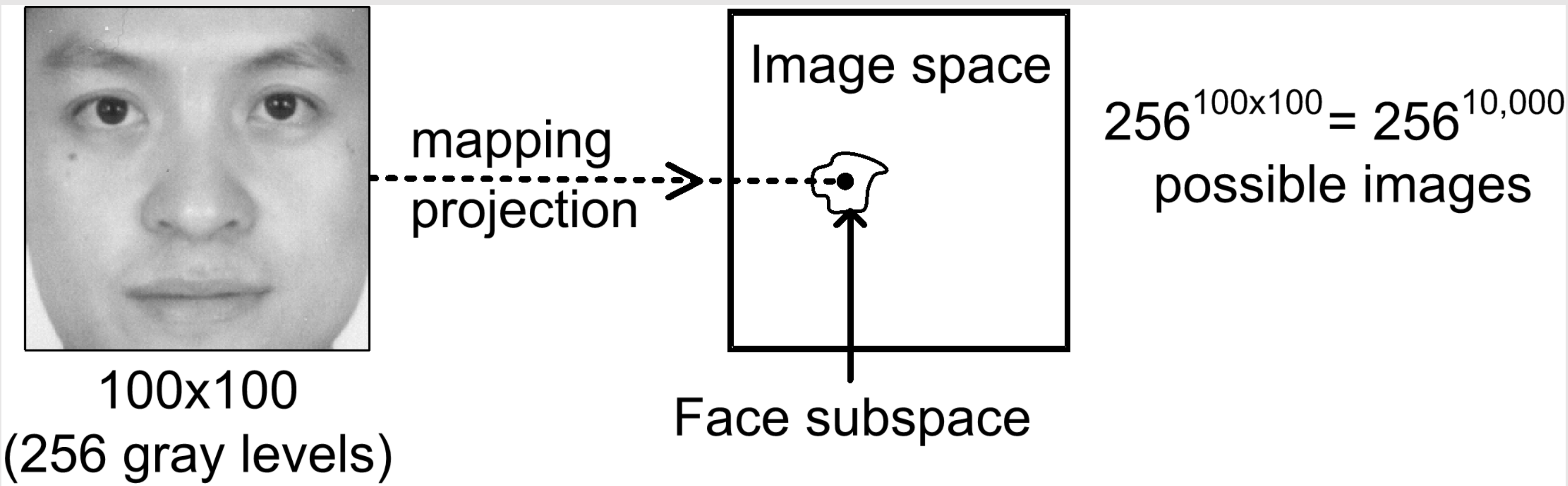
Question

- USPS dataset handwritten digit
- Size: 64 x 57; binary (1-bit, BW)
- The binary image space contains much more than just this digit.

How many possible images of this size and bit depth?

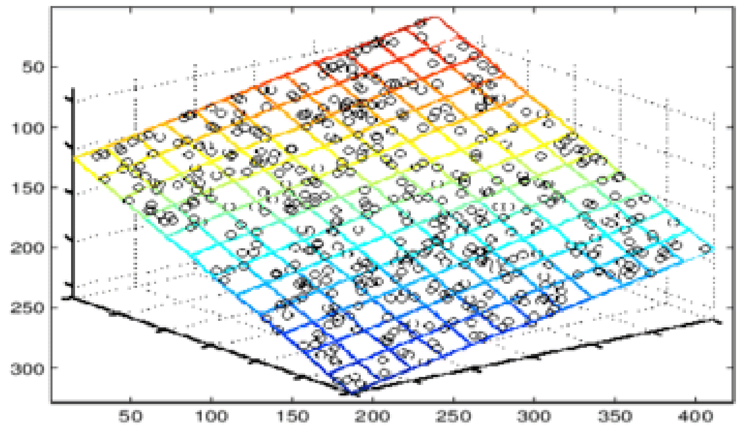
$$2^{64\times 57} = 2^{3648} = ?$$

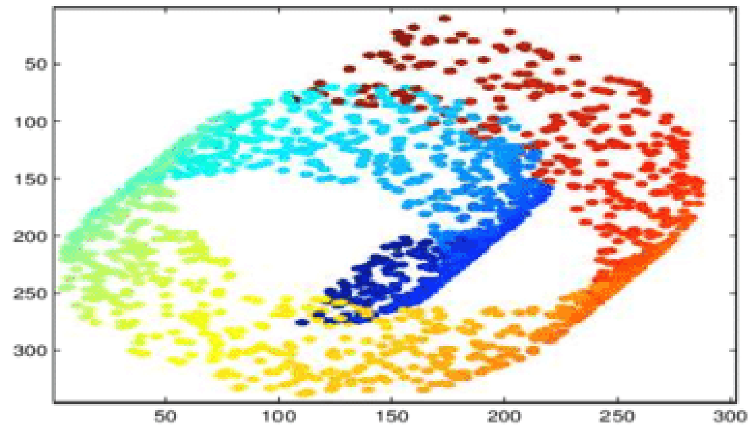
How About a Face?



Low-D Subspace/Manifolds

- For high dimensional data with **structure**:
  - Fewer variations than dimensions
  - Data to live on a lower dimensional manifold
  - → Deal with them by looking for a lower dimensional embedding (or projection, transformation)





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- Why Unsupervised Learning?
- **Principal Component Analysis (PCA)**
- PCA Unboxing
- Clustering: from k-means to spectral
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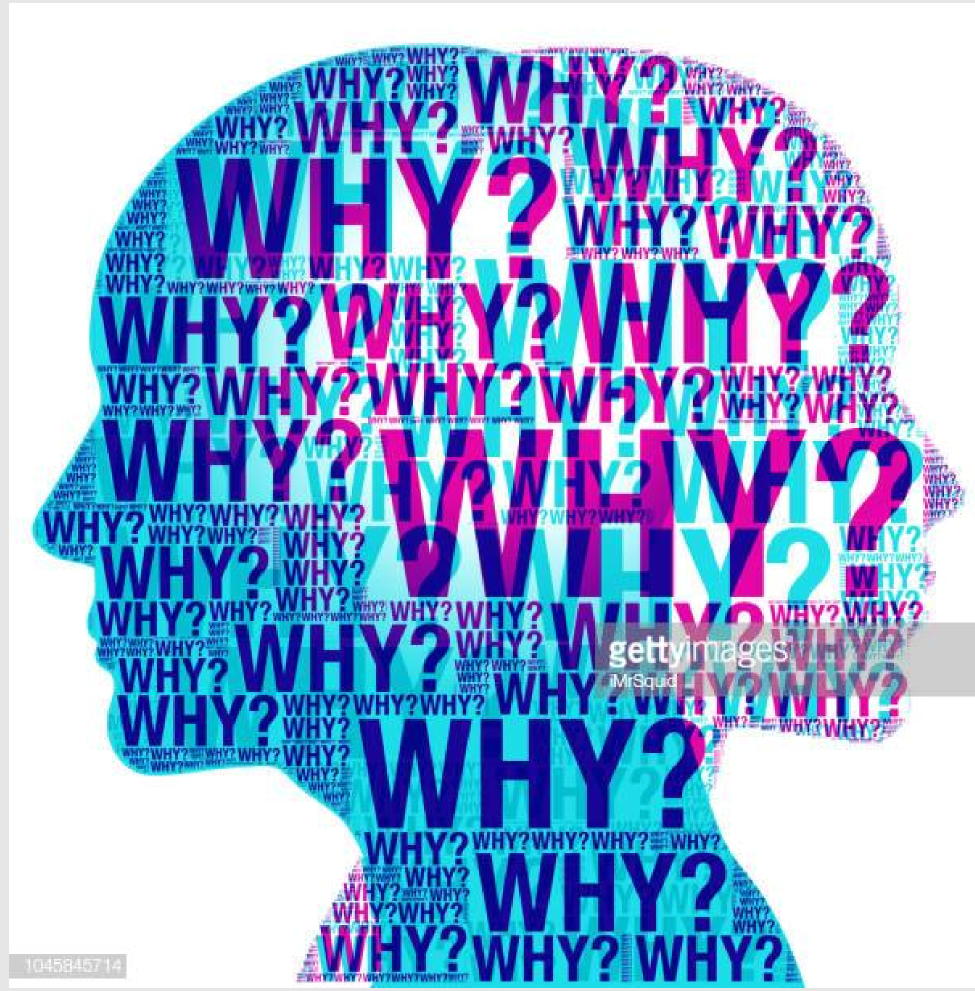
PCA?

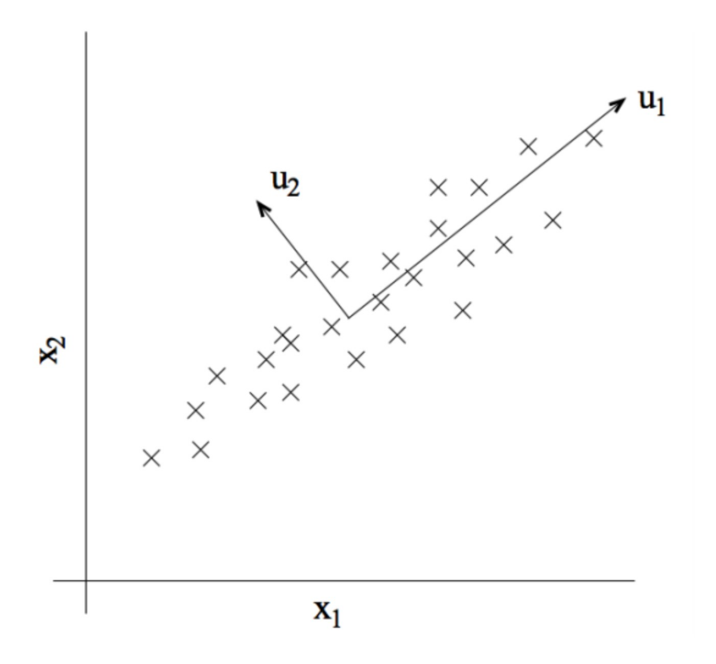
[Visualisation demo]



Principal Component Analysis

The idea:

1. Rotate the data with some rotation matrix **R** (change of basis) so that the new features are **uncorrelated**
2. Keep the dimension with the highest **variance** for DR



Principal Component Analysis

- PCA (@Hotelling:analysis33): a linear embedding
- Rotate to find *directions* in data with **maximum variance**
- How do we find these directions?
    - Diagonalize the **sample covariance** (**scatter**) **matrix** of N samples $\{\mathbf{x}^{(i)}, i = 1, \cdots, N\}$

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

Principal Component Analysis

- Given data $\{\mathbf{x}^{(i)}\}$, PCA finds **orthogonal** directions defined by a projection (rotation) $\mathbf{U}$ capturing the **maximum variance** in the data
- Solution: eigenvectors of $\mathbf{S}$ → $\mathbf{U}$
- PCA representation $\mathbf{y} = \mathbf{U}^\top \mathbf{x}$
- **Question**: Given the PCA representation $\mathbf{y}$, how to obtain an approximation/reconstruction of $\mathbf{x}$?

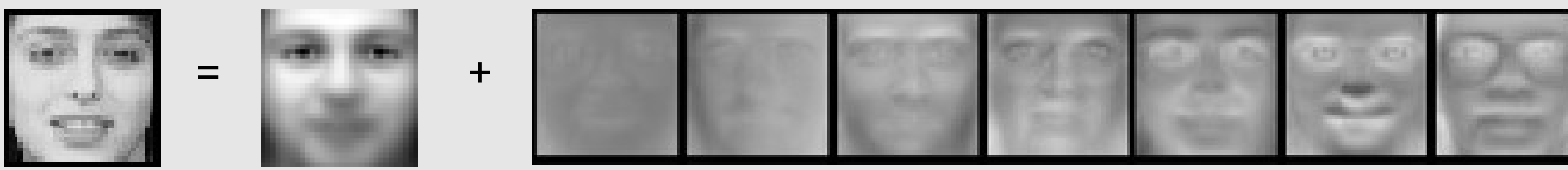
$$\hat{\mathbf{x}} = \mathbf{U}\mathbf{y}$$

Representation & Reconstruction

- Face $\mathbf{x}$ in k “face space” coordinates

$$\mathbf{x} \rightarrow [\mathbf{u}_1^\top(\mathbf{x}-\boldsymbol{\mu}), \cdots, \mathbf{u}_k^\top(\mathbf{x}-\boldsymbol{\mu})]$$
$$= [w_1, \cdots, w_k]$$

- Reconstruction: eigenvectors as orthonormal basis vectors



$$\hat{\mathbf{x}} \quad = \quad \boldsymbol{\mu} \quad + \quad w_1\mathbf{u}_1 + w_2\mathbf{u}_2 + w_3\mathbf{u}_3 + w_4\mathbf{u}_4 + \cdots$$

slide by Derek Hoiem

Reconstruction

$k = 4$

$k = 200$

$k = 400$

After computing eigenfaces using 400 face images from the ORL face database

slide by Derek Hoiem

PCA Ingredients

- **Data**: +pre-processing, e.g., $\mathcal{N}(0,1)$
- **Model**
  - Structure/Architecture: linear projection $\mathbf{y} = \mathbf{U}^\top \mathbf{x}$
  - **Hyper-parameter**: lower dimension k
  - Parameters (theta): the principal components (eigenvectors)
- Evaluation metric: max variance
- Optimisation: eigen-decomposition

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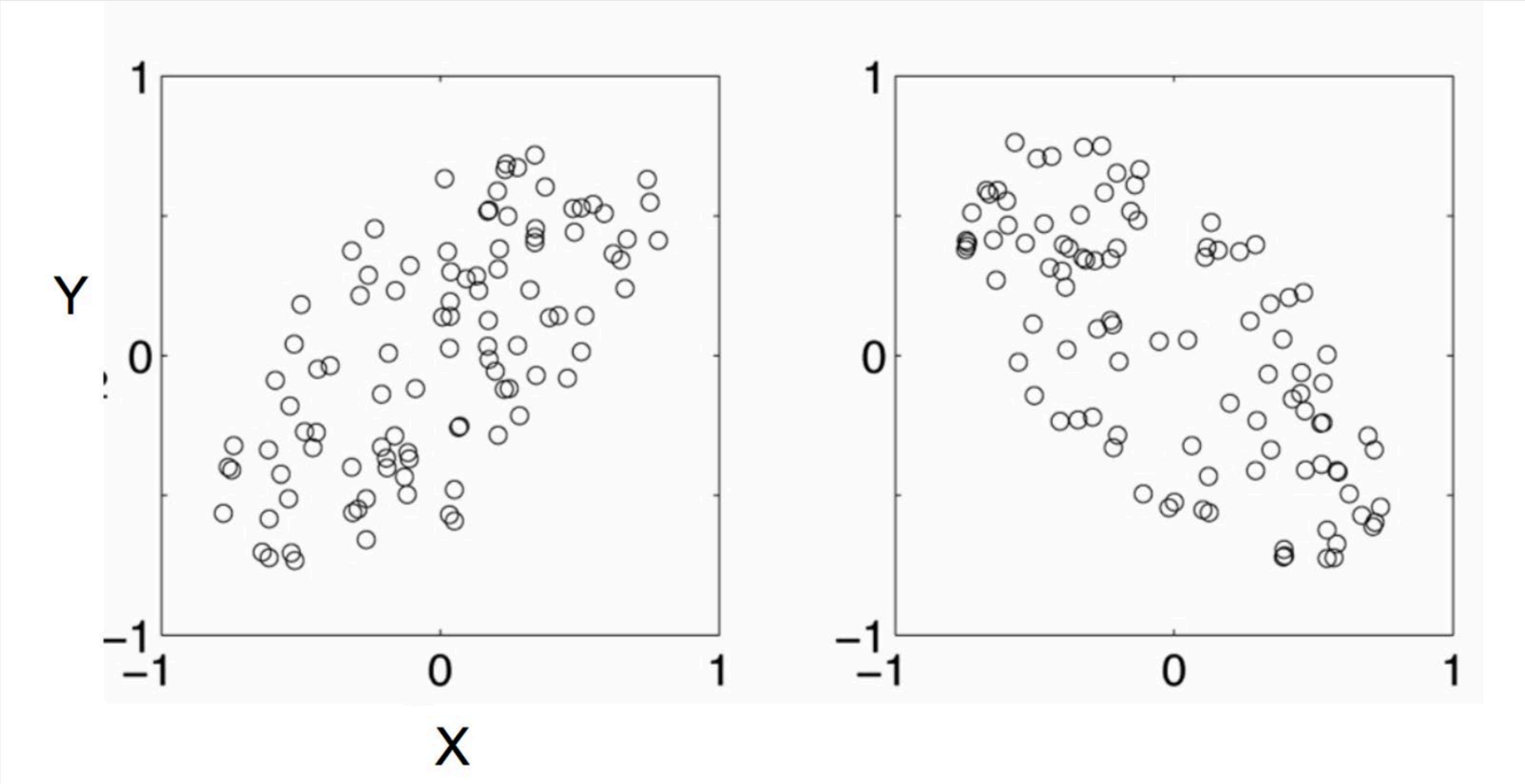
Variance →Covariance (Matrix)

- Variance and covariance:
  - Measure of the "spread" of a set of points around their *center of mass* (mean)
- Variance (scalar): scalar and matrix
  - Measure of the deviation from the mean for points in **one dimension**
- Covariance (**matrix**):
  - Measure of how much each of the dimensions vary from the mean with **respect to each other**

- Covariance is measured between two dimensions
- Covariance sees if there is a **relation** between the two dimensions
- Covariance between one dimension is the variance (degeneration)

Positive/Negative Covariance



Positive: Both dimensions increase or decrease together

Negative: While one increase the other decrease

Covariance Matrix

- Find relationships between dimensions in high dimensional data sets $\mathbf{X}$

plot

- Scatter matrix $\mathbf{S}$: sample-based estimation of covariance matrix (i: sample; j/k: variable)

$$s_{jk} = \frac{1}{N}\sum_{i=1}^{N}(X_{ij} - E(X_j))(X_{ik} - E(X_k))$$

The Sample mean

- Uncorrelated variables → covariance = 0
- Diagonal covariance mat → all variables are uncorrelated

keep the informations

PCA Derivation – Max Variance

- Scatter mat for the input $\mathbf{S} = \frac{1}{N}\sum_{i=1}^{N}\left(\mathbf{x}^{(i)} - \boldsymbol{\mu}\right)\left(\mathbf{x}^{(i)} - \boldsymbol{\mu}\right)^\top$
- **Question**: what is the scatter mat for the projections?

$$\mathbf{U}^\top \mathbf{S} \mathbf{U}$$

- First PC: **maximise the variance** in the **projected** space, i.e. the variance of $y = \mathbf{u}_1^\top \mathbf{x}$

$$\begin{aligned}\mathrm{var}(y) &= \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \mu_y\right)^2 \\ &= \frac{1}{N}\sum_{i=1}^{N}\mathbf{u}_1^\top\left(\mathbf{x}^{(i)} - \boldsymbol{\mu}_\mathbf{x}\right)\left(\mathbf{x}^{(i)} - \boldsymbol{\mu}_\mathbf{x}\right)^\top \mathbf{u}_1 \\ &= \mathbf{u}_1^\top \mathbf{S} \mathbf{u}_1\end{aligned}$$

PCA: Max Variance → Eigenvalue

- Find the first direction $\mathbf{u}_1$ via a unit-norm constrained optimisation, using Lagrange multipliers:

$$L\left(\mathbf{u}_1, \lambda_1\right) = \mathbf{u}_1^\top \mathbf{S}\mathbf{u}_1 + \lambda_1\left(1 - \mathbf{u}_1^\top \mathbf{u}_1\right)$$

- Gradient w.r.t. $\mathbf{u}_1$: $\dfrac{\mathrm{d}L\left(\mathbf{u}_1, \lambda_1\right)}{\mathrm{d}\mathbf{u}_1} = 2\mathbf{S}\mathbf{u}_1 - 2\lambda_1\mathbf{u}_1$
- Set to 0 and rearrange: $\mathbf{S}\mathbf{u}_1 = \lambda_1\mathbf{u}_1$ → First PC
  - Eigenvalue problem
- **Question**: many solutions (eigen-pairs), which to choose?

$$\mathrm{var}(y) = \mathbf{u}^\top \mathbf{S}\mathbf{u} = \lambda\mathbf{u}^\top\mathbf{u} = \lambda$$

PCA Solution

- Further directions: **orthogonal** (uncorrelated) to the first and each others → top k eigenvectors of $\mathbf{S}$
  - Eigenvectors: basis functions, principal components
  - Eigenvalue: the **variance** captured respectively
- **Questions**
  - For $\mathbf{u}_1$, what if we do not have the unit-norm constraint?

$$L(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^\top \mathbf{S} \mathbf{u}_1 + \cancel{\lambda_1 \left(1 - \mathbf{u}_1^\top \mathbf{u}_1\right)}$$

  →Trivial solution: infinity

  - For further directions: what if we do not require them to be orthogonal?

  → We will have the same $\mathbf{u}_1$, useless solution

PCA: Max Variance ←→ Min MSE

principle — mean-square error

Consider the first PC with the projection vector **u**. We assume **zero-mean**, i.e. *centered* data

Maximum Variance Direction: 1st PC = a vector **u** such that projection on it captures max variance in the data

$$\frac{1}{N}\sum_{i=1}^{N}(\mathbf{u}^T\mathbf{x}^{(i)})^2 = \mathbf{u}^T\mathbf{X}\mathbf{X}^T\mathbf{u}$$

Minimum Reconstruction Error: 1st PC = a vector **u** such that projection on it yields minimum MSE reconstruction

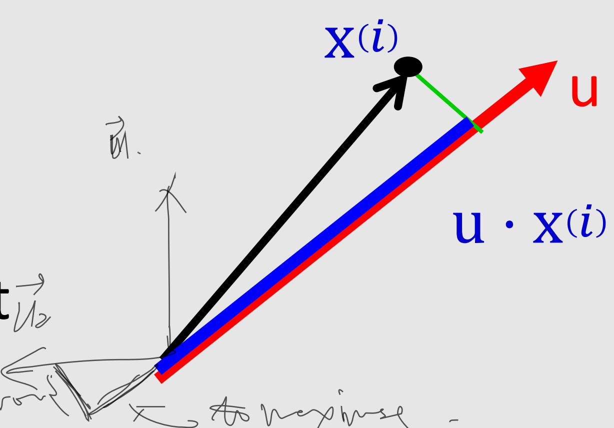
$$\frac{1}{N}\sum_{i=1}^{N}\|\mathbf{x}^{(i)} - (\mathbf{u}^T\mathbf{x}^{(i)})\mathbf{u}\|^2$$

error

blue^2 + green^2 = black^2

black^2 is fixed (it's just the data)

So, maximizing blue^2 is equivalent to minimizing green^2



How many (k) PCs to keep?

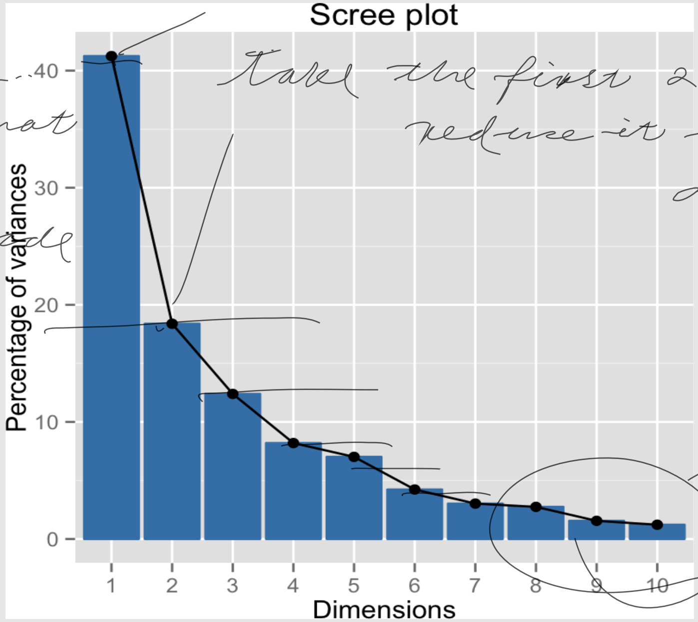
principle components

- Pick based on percentage of variance captured / lost
  - Variance captured: the variance of the projected data
  - Pick smallest k that explains a certain percentage of variance

(Sum of first k EVs)/(sum of all EVs)

- Look for an "elbow" in scree plot (plot of explained variance or eigenvalues)

variance indicates that information is inside



Take the first 2 to reduce it to 2-d dataset.

variance

after rotated vector

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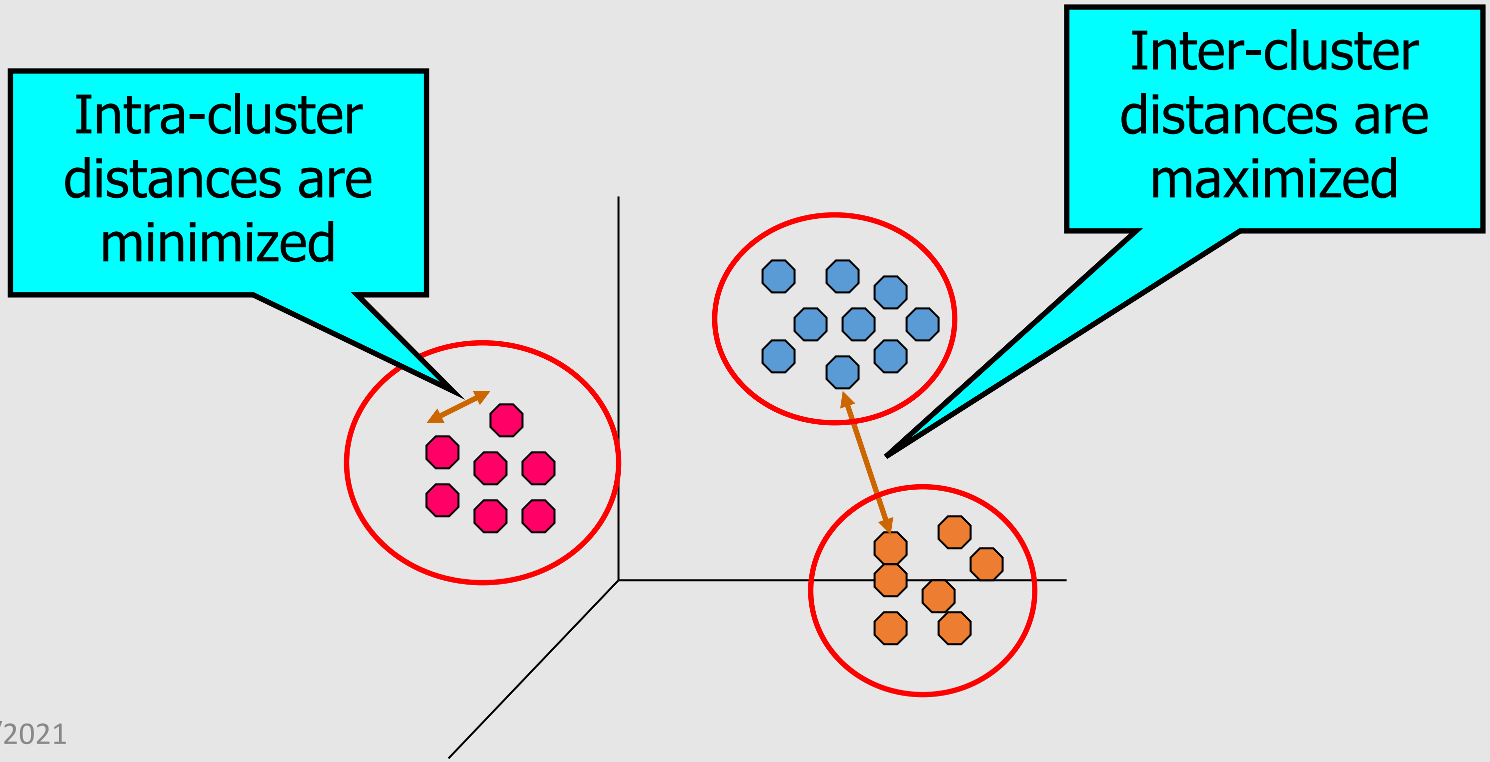
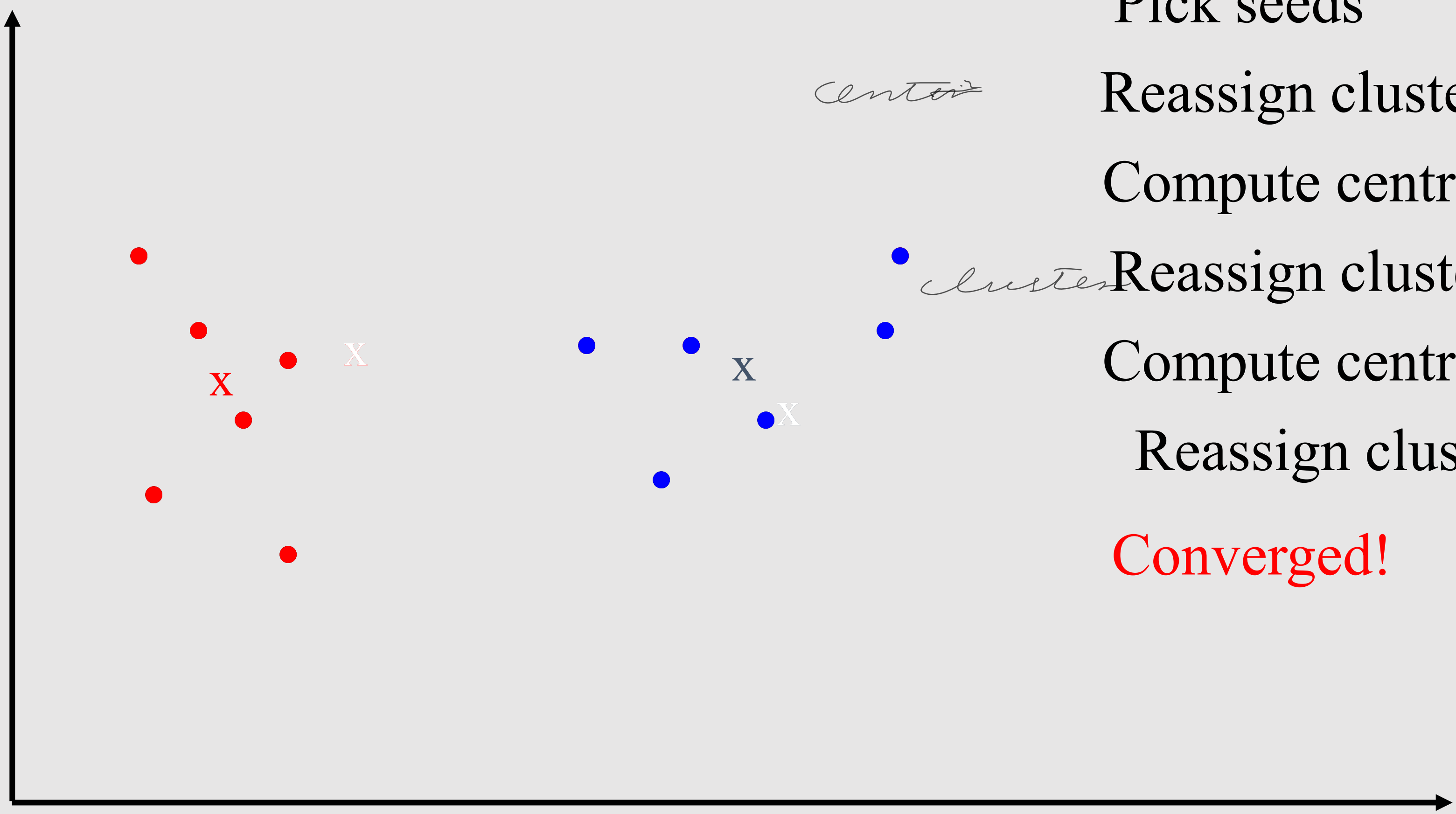
What is Clustering?

define a metric to seperate clusters/boundaries

- Find grouping of objects such that the objects in a group will be similar or more related to one another and those in different groups will be different or less related



k-means Example (*k*=2)



Pick seeds

Reassign clusters

Compute centroids

Reassign clusters

Compute centroids

Reassign clusters

Converged!

They will create labels based on algorithm

Machine Learning	Supervised	Unsupervised
Discrete output	Classification	Clustering
Continuous output	Regression	Dimensionality Reduction

labels included

k-means & PCA

Reduce into a algorithm-generated label.

- The objective of k-means clustering: to minimize the within-cluster scatter

j - center to minimize variance ?

$$\min \sum_{j=1}^{k} \sum_{i \text{ allocated to } j} \left(\mathbf{x}^{(i)} - \boldsymbol{\mu}^{(j)}\right)^\top \left(\mathbf{x}^{(i)} - \boldsymbol{\mu}^{(j)}\right)$$

- Similarity with PCA: also measure of the “spread” of a set of points around their *center of mass* (mean)
- Clustering analogy
  - Classification w/o labelled training data
  - Extreme dimensionality reduction (to a **cluster label**)

k-means Clustering Ingredients

- **Data**: +pre-processing, e.g., $\mathcal{N}(0,1)$
- **Model**

  different clusters

  - Structure/Architecture: linear separation btw clusters
  - **Hyper-parameter**: #clusters k

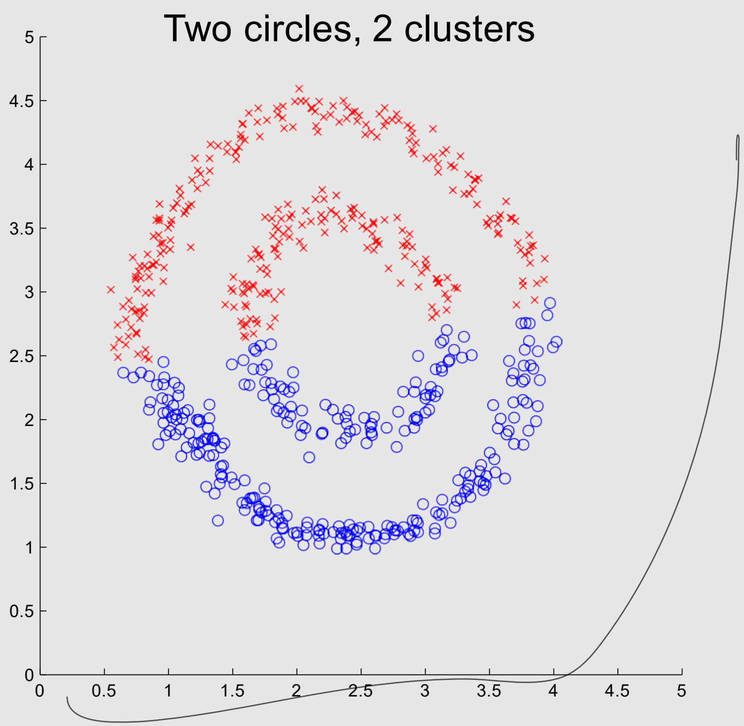
    θ
  - Parameters (theta): the k cluster centroids

  to learn which parameter will seperate the clusters with the maximum variance
- Evaluation metric: within-cluster scatter
- Optimisation: expectation maximisation (EM), kind of gradient descent

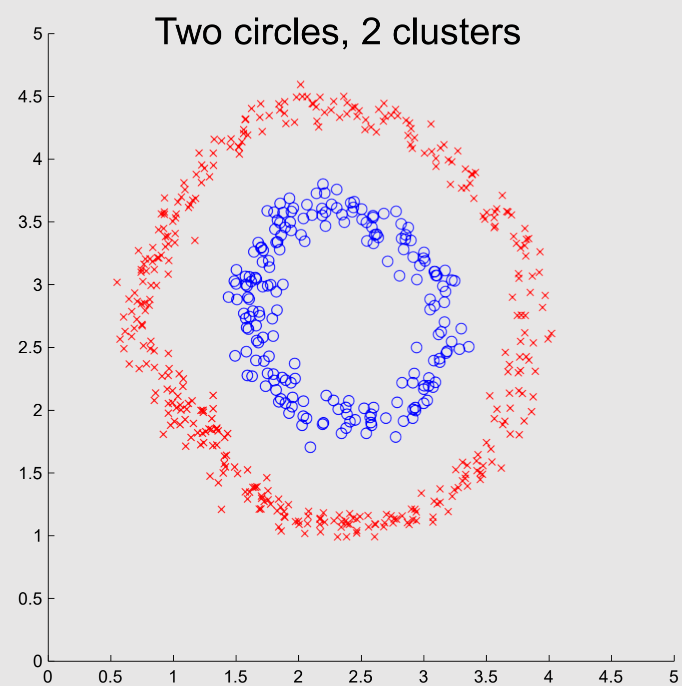
k-means Has a Problem

- k-means: centroid-based, for compactness (scatter)
- Spectral clustering: **connectivity**

k-means



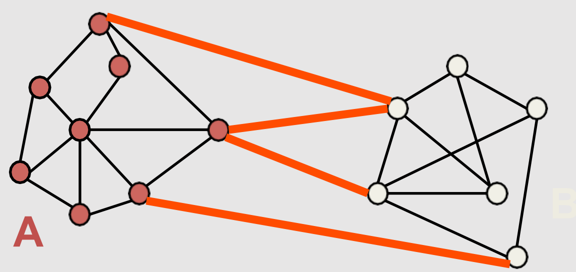
Spectral clustering

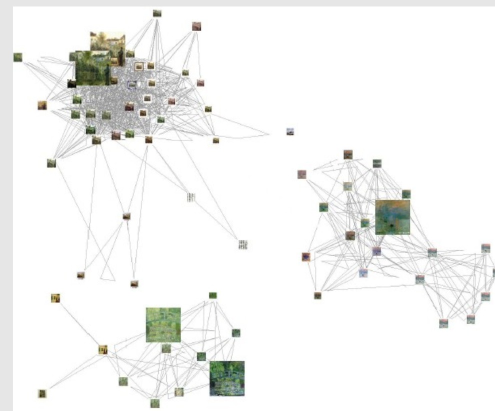


[Shi & Malik ‘00; Ng, Jordan, Weiss NeurIPS ‘01]

Spectral Clustering

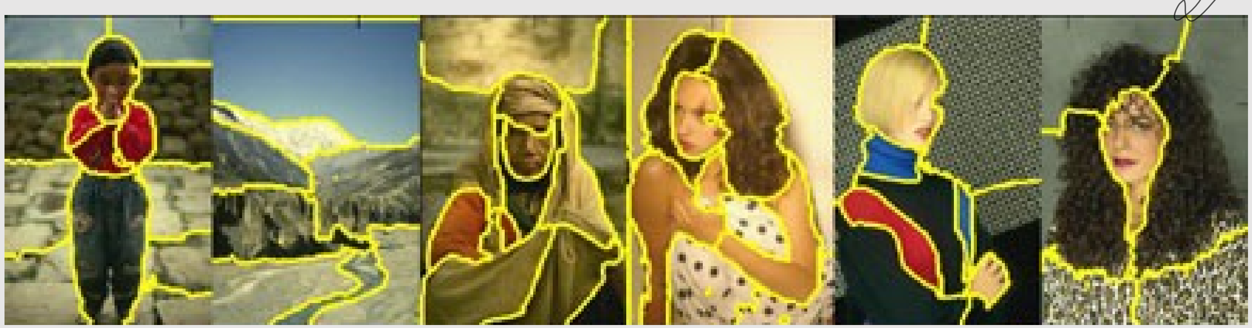
- Group points based on **links** in a **graph**





- Image as graph: segmentation as clustering

connectivity



Slide from James Hays

How to Create the Graph?

- Gaussian kernel→ compute similarity between objects

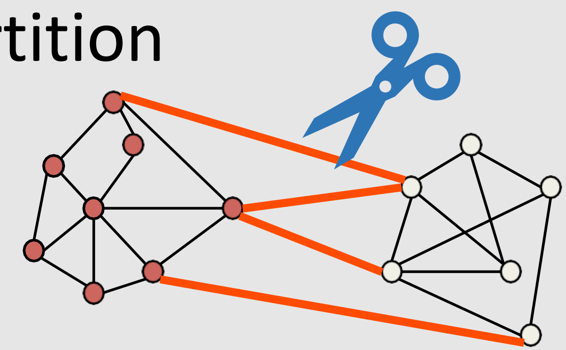
$$\mathbf{W}(i,j) = \exp \frac{-|x_i - x_j|^2}{\sigma^2} \quad e^{\cdots}$$

- One could create
  - A fully connected graph (~ FC layer)
  - K-nearest neighbour graph: each node is only connected to its K-nearest neighbours (~ convolutional layer, local connectivity)

the most similar

e.g. social network

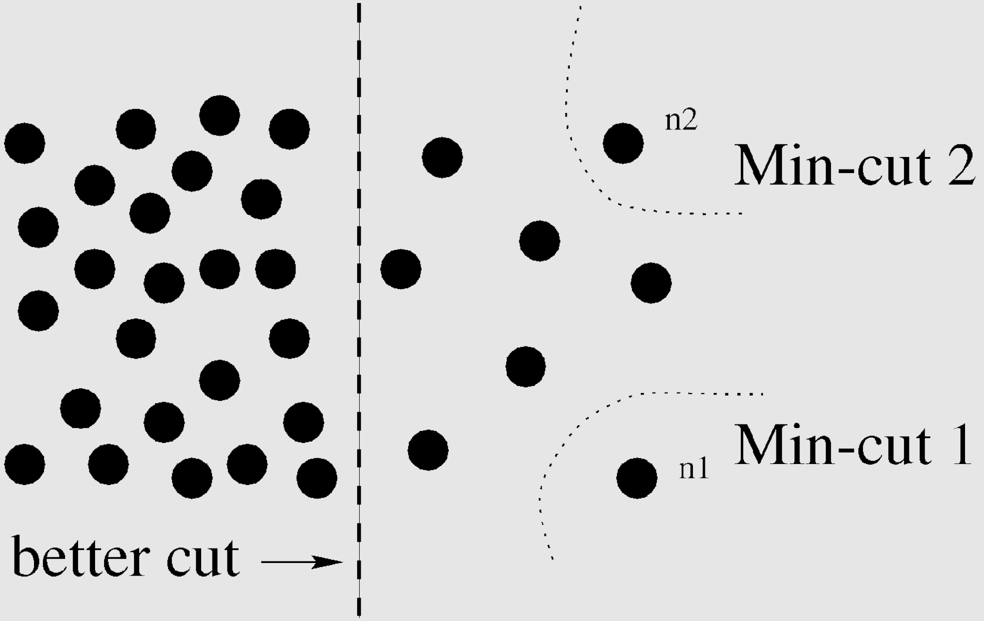
- Clustering → Graph cut/partition
  - Objective: **minimise** cut



Slide from Alan Fern

Min Cut = Good Cut?

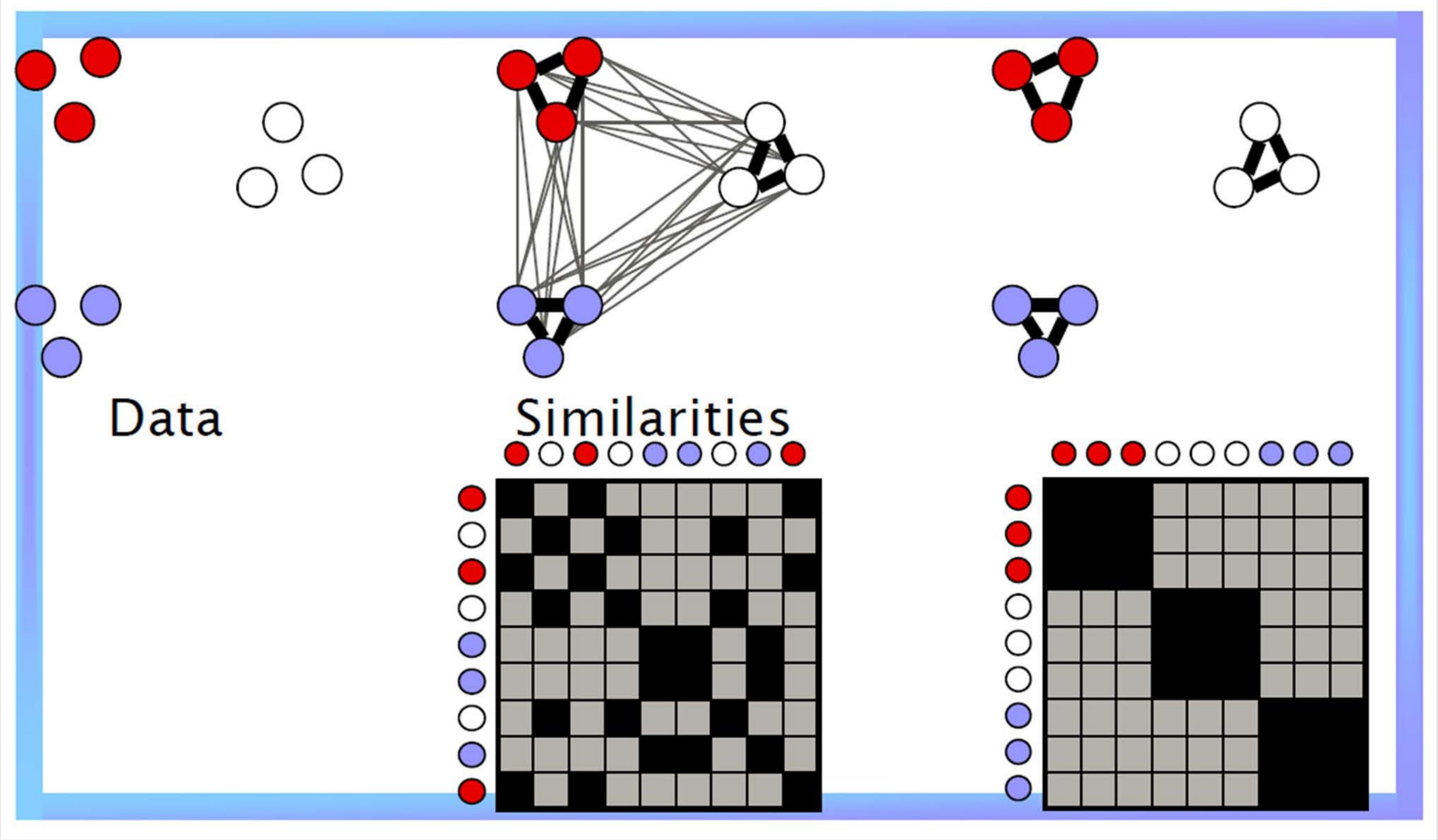
- A case where minimum cut gives a bad partition



- Solution: **Normalise** the cut

[Shi & Malik ‘00]

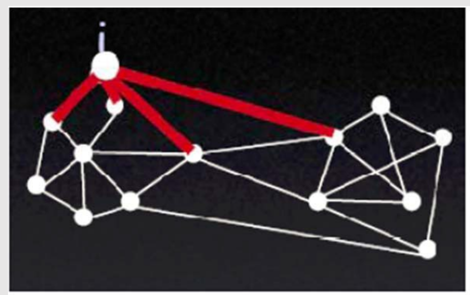
Graph Clustering Process

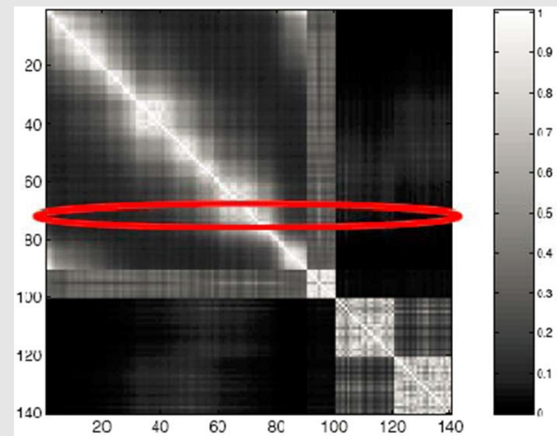


Graph Terminologies

- Degree of nodes

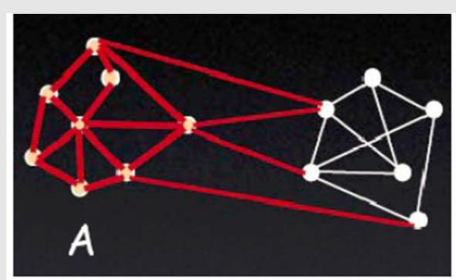
$$d_i = \sum_j w_{i,j}$$

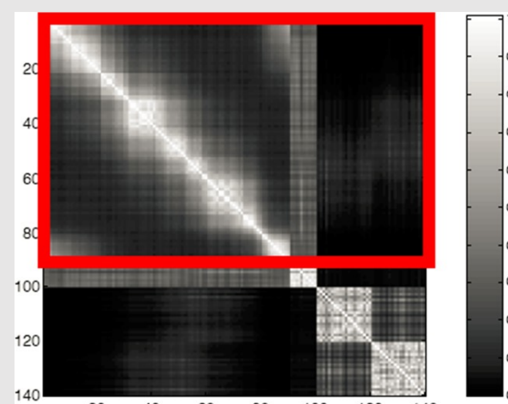




- Volume of a set

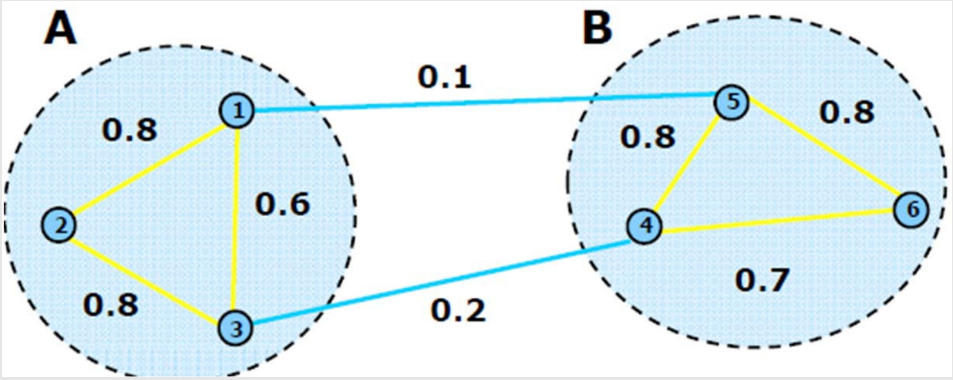
$$vol(A) = \sum_{i \in A} d_i, A \subseteq V$$





Graph Cut

- Consider a partition of the graph into two parts *A* & *B*



Question

$$cut(A, B) =$$

- $cut(A, B)$: sum of the weights of the set of edges that connect the two groups

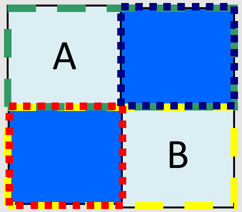
$$cut(A, B) = \sum_{i \in A, j \in B} w_{ij}$$

- Goal: find the partition that minimizes the cut

Normalized Cut (Ncut)

- Consider the **connectivity** between groups **relative** to the volume of each group

$$Ncut(A,B) = \frac{cut(A,B)}{Vol(A)} + \frac{cut(A,B)}{Vol(B)}$$



$$Ncut(A,B) = cut(A,B)\frac{Vol(A)+Vol(B)}{Vol(A)Vol(B)}$$

\usepackage{mathtools}

Solving/Minimising Ncut

- Compute the similarity matrix $\mathbf{W} : \mathbf{W}(i,j) = w_{i,j}$
- Compute the degree matrix $\mathbf{D} : \mathbf{D}(i,i) = \sum_j w_{i,j}$
- Solve a generalised **eigenvalue** problem (relaxed Ncut)

$$\min_{\mathbf{y}} \mathbf{y}^\top (\mathbf{D} - \mathbf{W})\mathbf{y} \text{ s.t. } \mathbf{y}^\top \mathbf{D}\mathbf{y} = 1 \Rightarrow (\mathbf{D} - \mathbf{W})\mathbf{y} = \lambda \mathbf{D}\mathbf{y}$$

(D-W) : Laplacian matrix

- Solution:
  - Bipartition: use the eigenvector with the second smallest eigenvalue to partition the graph into two parts
    - Splitting point: minimum Ncut (plot). all the point in the graph.
  - K-way partition: *k*-means clustering of multiple eigenvectors
    - Graph embedding (dimensionality reduction) → eigenvectors

Recap: Power of Transform

- Logistic regression **transforms** classification into linear regression of the log odds, modelling the probability of the predicted output rather than the output itself.
- Spectral clustering **transforms** non-linear clustering into (linear) k-means clustering of generalised eigenvectors based on the similarity graph, modelling the connectivity of data points rather than themselves.

https://i.kym-cdn.com/photos/images/newsfeed/001/030/448/b9f.gif

Spectral Clustering Ingredients

- **Data**: +pre-processing, e.g., $\mathcal{N}(0,1)$
- **Model**
  - Structure/Architecture: spectral (nonlinear) separation btw clusters
  - **Hyper-parameter**: #clusters k (+#eigenvectors), kernel bandwidth σ
  - Parameters (theta): the (generalised) eigenvectors
- Evaluation metric: normalised (graph) cut
- Optimisation: eigen-decomposition (and expectation maximisation in k-means)

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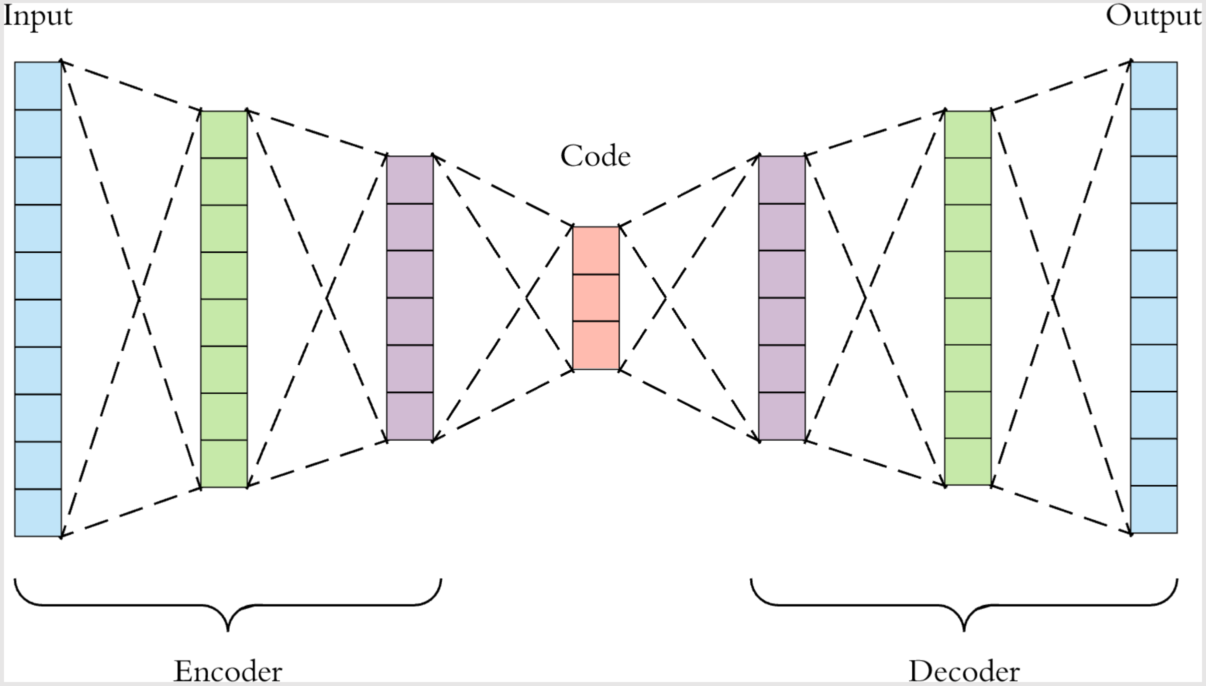
- Clustering: from k-means to spectral
- **Autoencoder**

Autoencoder

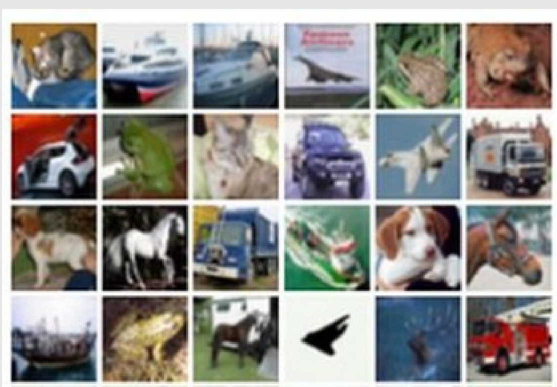
- **Encoder:** compress data or extract features
- **Decoder:** generate images given a new code
- **Bottleneck** (**code**): to make it non-trivial, much smaller dimension as the latent representation

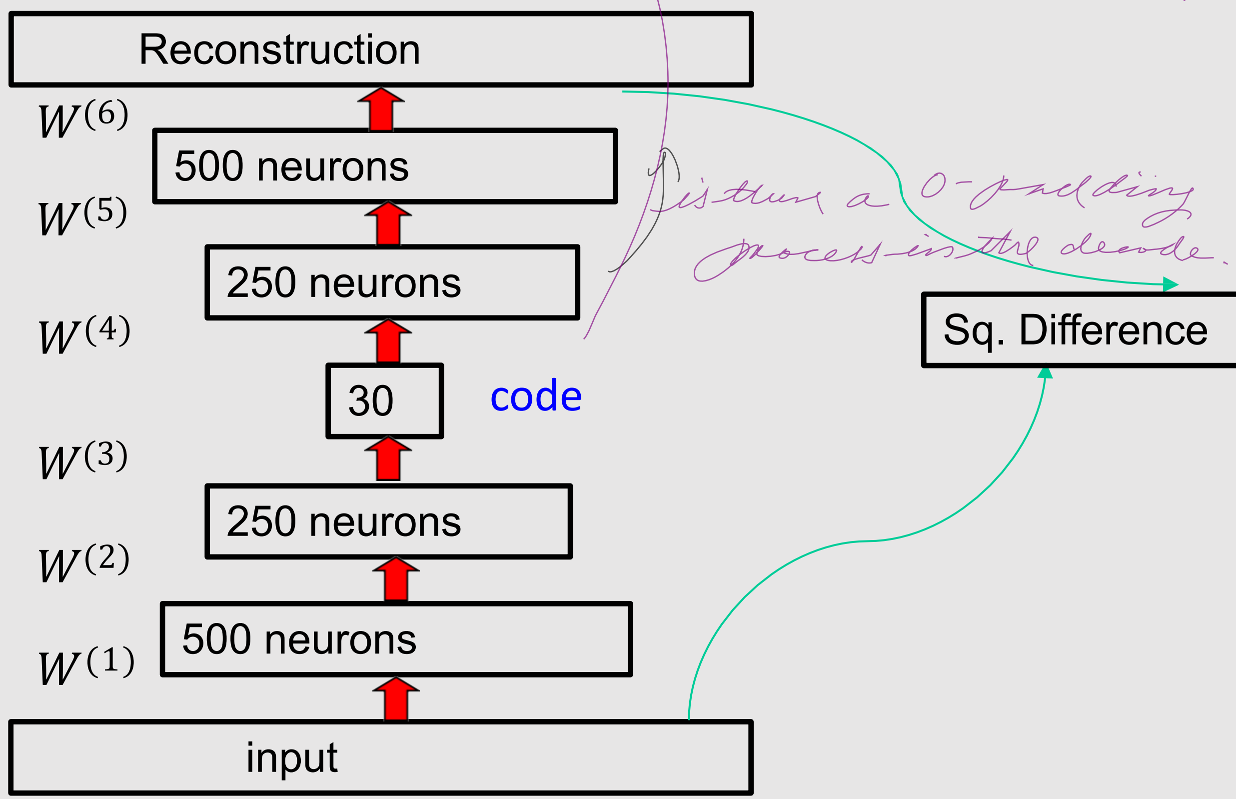


https://miro.medium.com/max/3148/1*44eDEuZBEsmG_TCAKRI3Kw@2x.png

Autoencoder Example

expand the data with what.



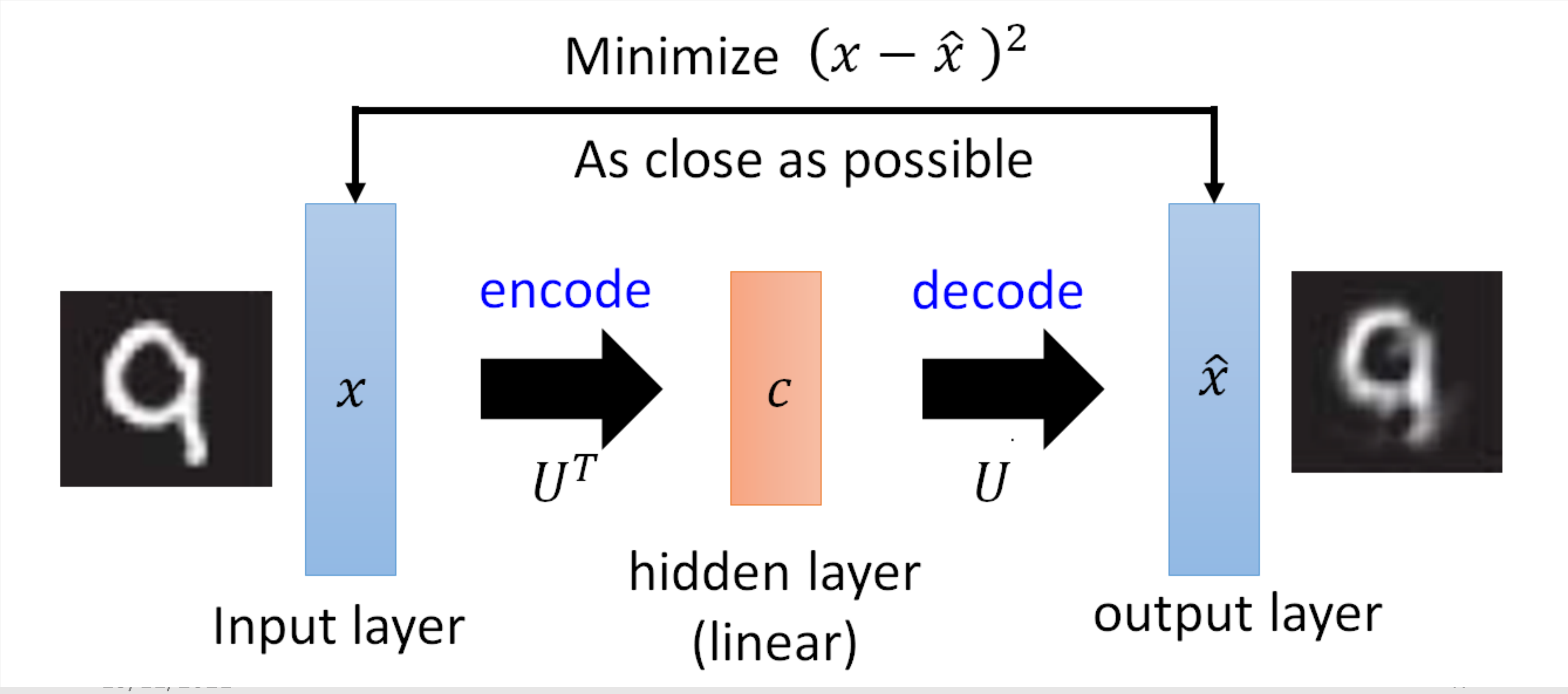


is there a 0-padding process in the decode.

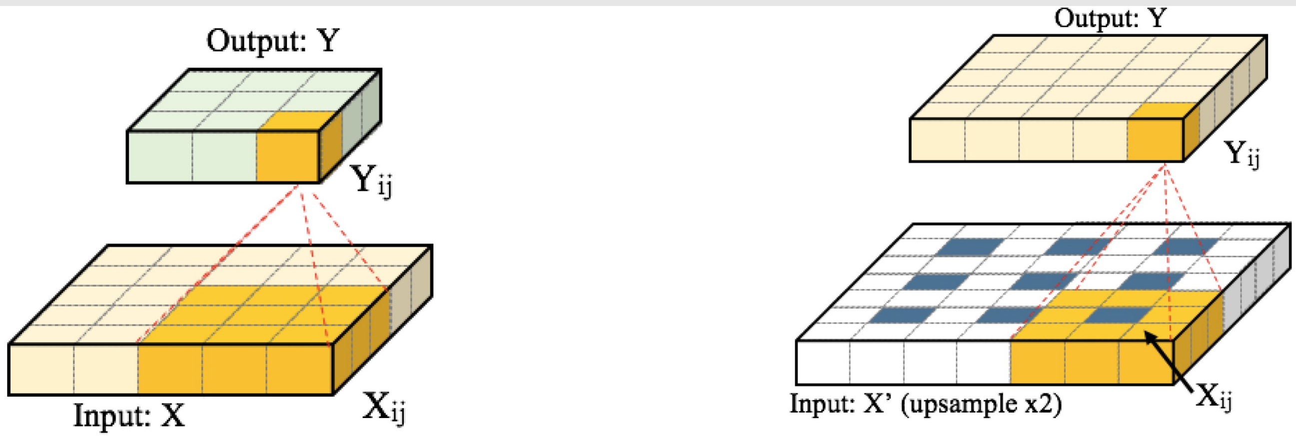
- Find the weights minimising the difference between the input and reconstruction
- The code layer (bottleneck) is a low--dimensional summary of the input

PCA as Linear Autoencoder

- PCA: autoencoder w/t single-layer encoder/decoder
- Weight sharing between the encoder and decoder



Transpose Convolution Layer



(**a**) Convolutional layer: the input size is $W_1 = H_1 = 5$; the receptive field $F = 3$; the convolution is performed with stride $S = 1$ and no padding ($P = 0$). The output Yis of size $W_2 = H_2 = 3$.

(**b**) Transposed convolutional layer: input size $W_1 = H_1 = 3$; transposed convolution with stride $S = 2$; padding with $P = 1$; and a receptive field of $F = 3$. The output Yis of size $W_2 = H_2 = 5$.

https://www.mdpi.com/2072-4292/9/6/522/htm

More at https://github.com/vdumoulin/conv_arithmetic

Convolutional Autoencoder (Lab)

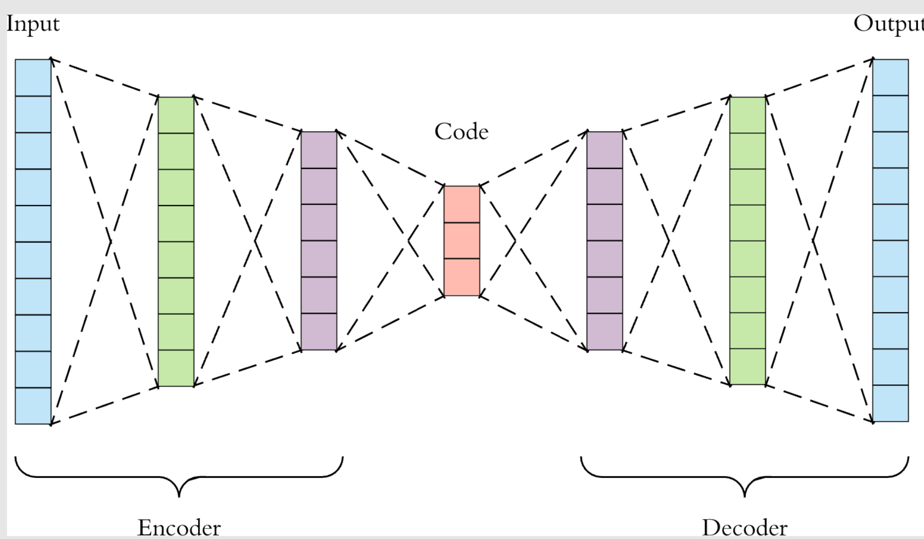
```
class Autoencoder(nn.Module):
    def __init__(self):
        super(Autoencoder, self).__init__()
        self.encoder = nn.Sequential(
            # 1 input image channel, 16 output channel, 3x3 square convolution
            nn.Conv2d(1, 16, 3, stride=2, padding=1),
            nn.ReLU(),
            nn.Conv2d(16, 32, 3, stride=2, padding=1),
            nn.ReLU(),
            nn.Conv2d(32, 64, 7)
        )
        self.decoder = nn.Sequential(
            nn.ConvTranspose2d(64, 32, 7),
            nn.ReLU(),
            nn.ConvTranspose2d(32, 16, 3, stride=2, padding=1, output_padding=1),
            nn.ReLU(),
            nn.ConvTranspose2d(16, 1, 3, stride=2, padding=1, output_padding=1),
            nn.Sigmoid()  #to range [0, 1]
        )

    def forward(self, x):
        x = self.encoder(x)
        x = self.decoder(x)
        return x
```

Training

Sample labeled data (**batch**) → **Forward** it through the network, get predictions → **Back-propagate** the errors → **Update** the network weights

Data → Model → Metric → Optimisation



Autoencoder Ingredients

- **Data**: + pre-processing, e.g., $\mathcal{N}(0,1)$
- **Model**
  - Structure/Architecture: layers defined in nn.module
  - **Hyper-parameter**: layer specs, e.g. #layers #channels, kernel size
  - Parameters (theta): layer weights and biases
- Evaluation metric: MSE or other
- Optimisation: backprop, SGD or the like

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Recommended Reading

- The PCA book (from a UIUC link)
- Chapter on PCA in most machine learning books
- Chapter on clustering in most machine learning books
- The normalized cut paper in 2000
- Chapter on autoencoder in the Deep Learning Book

- Wikipedia entries on covered topics
- Scikit-learn/PyTorch documentations
- The lab notebook and references