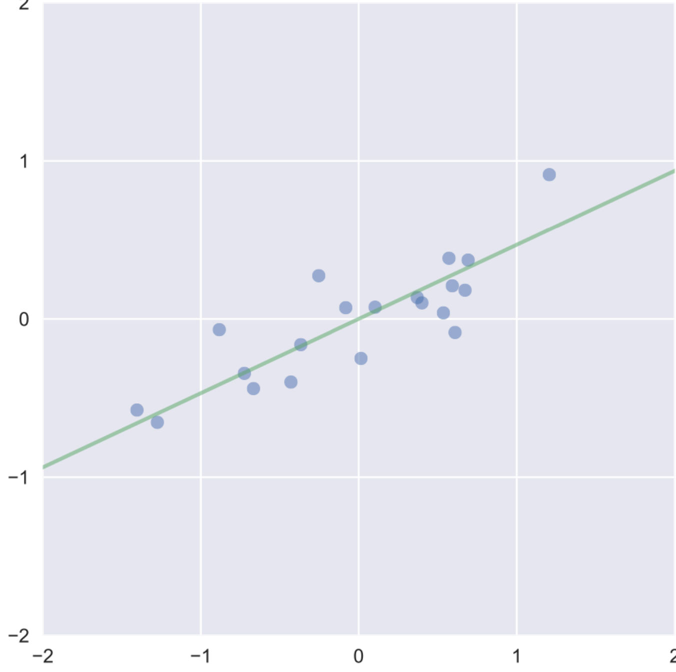


Lecture 23: Principal Component Analysis

- Unsupervised learning
  - Dimensionality reduction
    - **PCA**
    - **Auto-encoder**
  - Clustering
    - k-means
    - Spectral,t-SNE,UMAP
  - Generative models
  - Density estimation

The principal component analysis

- so far we considered finding ONE principal component $u \in \mathbb{R}^d$
- it is the eigenvector corresponding to the maximum eigenvalue of the covariance matrix
$$\mathbf{C} = \frac{1}{n}\mathbf{X}^T\mathbf{X} \in \mathbb{R}^{d \times d}$$
- We can also use the Singular Value Decomposition (SVD) to find such eigen vector
- note that is the data is not centered at the origin, we should re-center the data before applying SVD

- in general we define and use multiple principal components
- if we need r principal components, we take r eigenvectors corresponding to the largest r eigenvalues of $\mathbf{C}$

Algorithm: Principal Component Analysis

- **input**: data points $\{x_i\}_{i=1}^n$, target dimension $r \ll d$
- **output**: r-dimensional subspace U
- **algorithm**:
  - compute mean $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$
  - compute covariance matrix
    $$\mathbf{C} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})^T$$
  - let $(u_1, \ldots, u_r)$ be the set of (normalized) eigenvectors with corresponding to the largest r eigenvalues of $\mathbf{C}$
  - return $\mathbf{U} = [u_1 \quad u_2 \quad \cdots \quad u_r]$

- further the data points can be represented compactly via
  $$a_i = \mathbf{U}^T(x_i - \bar{x}) \in \mathbb{R}^r$$

How do we compute singular vectors?

- In practice: Lanczos method
- We will learn: power iteration
- Let $C = USU^T \in \mathbb{R}^{d \times d}$ be SVD of the matrix we want to compute the top one singular vector
  - $U = [u_1, u_2, \ldots, u_d]$ are the singular vectors (ordered in the decreasing order of the corresponding singular values)
  - We also assume $\lambda_1 > \lambda_2$ in order to ensure uniqueness of u_1

$$\tilde{v}_{t+1} \leftarrow Cv_t$$

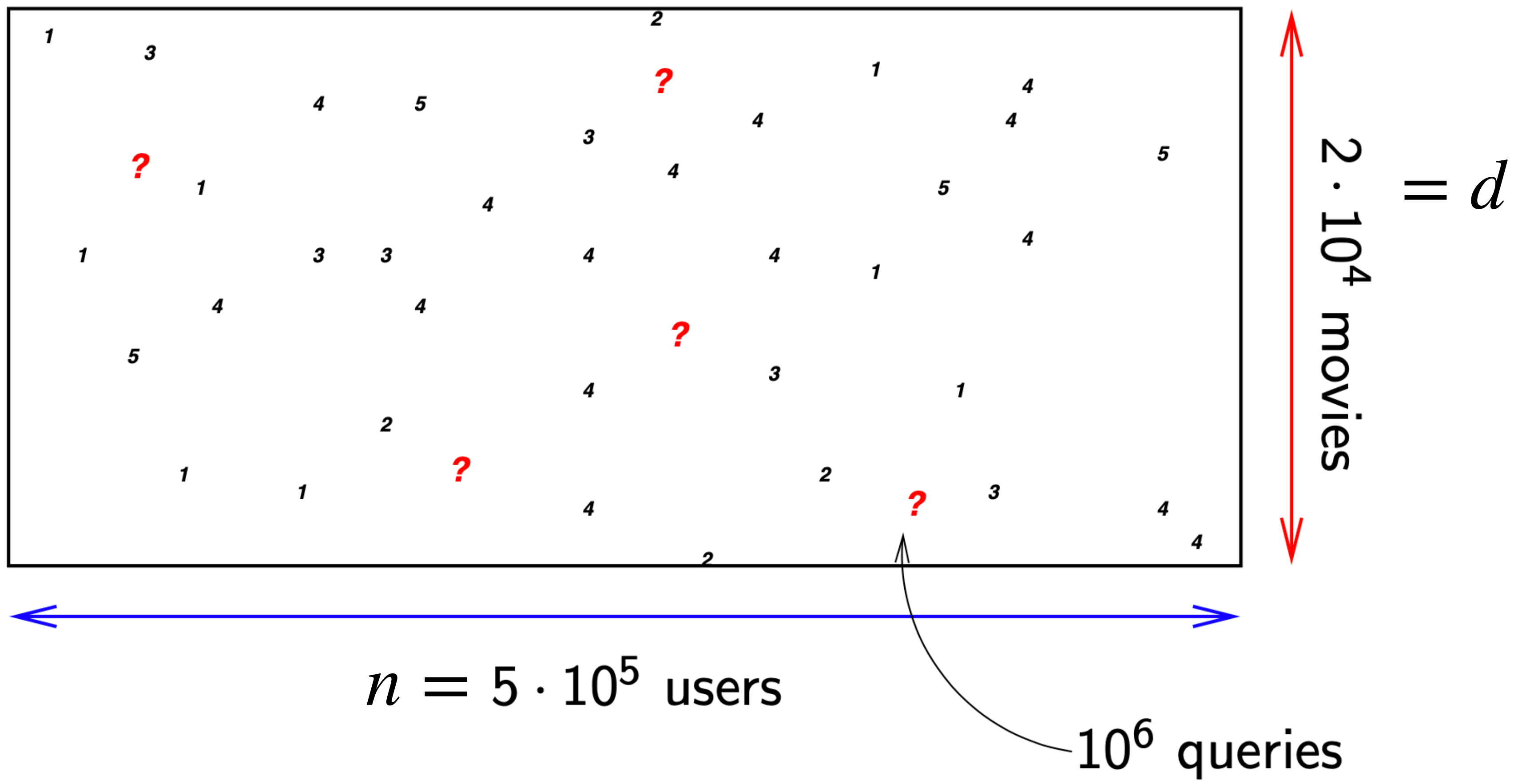
$$v_{t+1} \leftarrow \frac{\tilde{v}_{t+1}}{|\tilde{v}_{t+1}|}$$

Power iteration

$$\tilde{v}_{t+1} \leftarrow C v_t$$

$$v_{t+1} \leftarrow \frac{\tilde{v}_{t+1}}{|\tilde{v}_{t+1}|}$$

Matrix completion for recommendation systems



- users provide ratings on a few movies, and we want to predict the missing entries in this ratings matrix, so that we can make recommendations
- without any assumptions, the missing entries can be anything, and no prediction is possible

Matrix completion

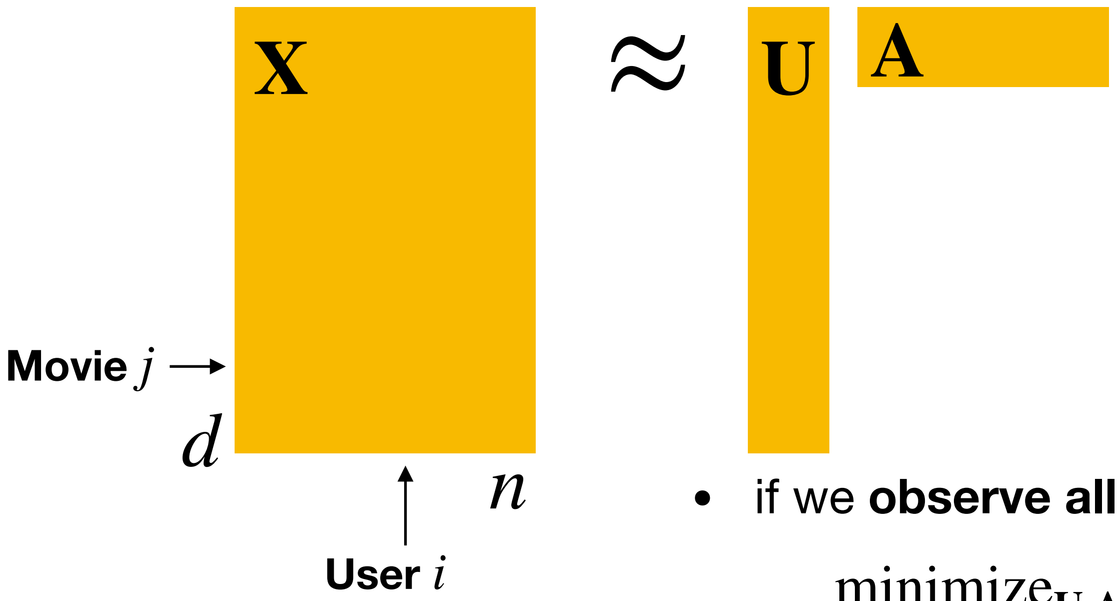
- however, the ratings are not arbitrary, but people with similar tastes rate similarly
- such structure can be modeled using low dimensional representation of the data as follows
- we will find a set of principal component vectors $\mathbf{U} = [u_1 \quad u_2 \quad \cdots \quad u_r] \; \in \mathbb{R}^{d \times r}$
- such that that ratings $x_i \in \mathbb{R}^d$ of user i, can be represented as

$$\begin{aligned} x_i &= a_i[1]u_1 + \cdots a_i[r]u_r \\ &= \mathbf{U}a_i \end{aligned}$$

  for some lower-dimensional $a_i \in \mathbb{R}^r$ for i-th user and some $r \ll d$
- for example, $u_1 \in \mathbb{R}^d$ means how horror movie fans like each of the d movies,
- and $a_i[1]$ means how much user i is fan of horror movies

Matrix completion

- let $\mathbf{X} = [x_1 \quad x_2 \quad \cdots \quad x_n] \in \mathbb{R}^{d \times n}$ be the ratings matrix, and assume it is fully observed, i.e. we know all the entries
- then we want to find $\mathbf{U} \in \mathbb{R}^{d \times r}$ and $\mathbf{A} = [a_1 \quad a_2 \quad \cdots \quad a_n] \in \mathbb{R}^{r \times n}$ that approximates $\mathbf{X}$



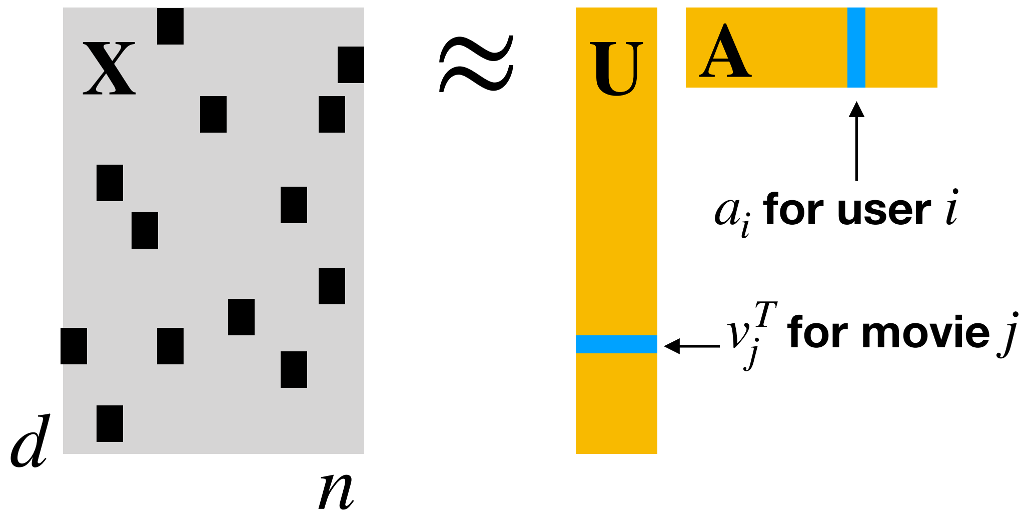
- if we **observe all entries** of $\mathbf{X}$, then we can solve

$$\text{minimize}_{\mathbf{U},\mathbf{A}} \sum_{i=1}^{n} \|x_i - \mathbf{U}a_i\|_2^2$$

which can be solved using PCA (i.e. SVD)

Matrix completion

- in practice, we only observe $\mathbf{X}$ partially
- let $S_{\text{train}} = \{(i_\ell, j_\ell)\}_{\ell=1}^{N}$ denote N observed ratings for user i_ℓ on movie j_ℓ



- let v_j^T denote the j-th row of $\mathbf{U}$ and a_i denote i-th column of $\mathbf{A}$
- then user i's rating on movie j, i.e. $\mathbf{X}_{ji}$ is approximated by $v_j^T a_i$, which is the inner product of v_j (a column vector) and a column vector a_i
- we can also write it as $\langle v_j, a_i \rangle = v_j^T a_i$

Matrix completion

- a natural approach to fit v_j's and $a_i's$ to given training data is to solve

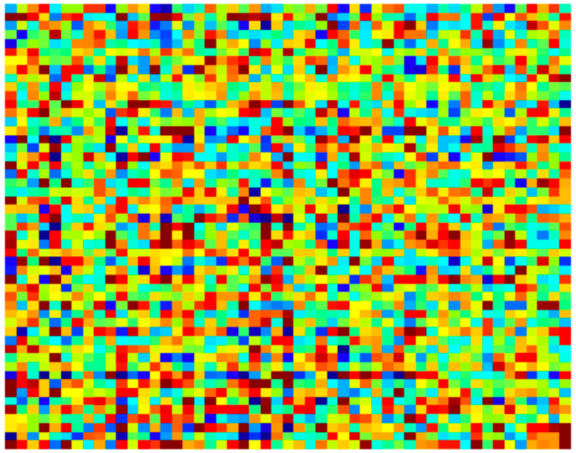
$$\text{minimize}_{\mathbf{U},\mathbf{A}} \sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} - v_j^T a_i)^2$$

- this can be solved, for example via gradient descent or alternating minimization
- this can be quite accurate, with small number of samples

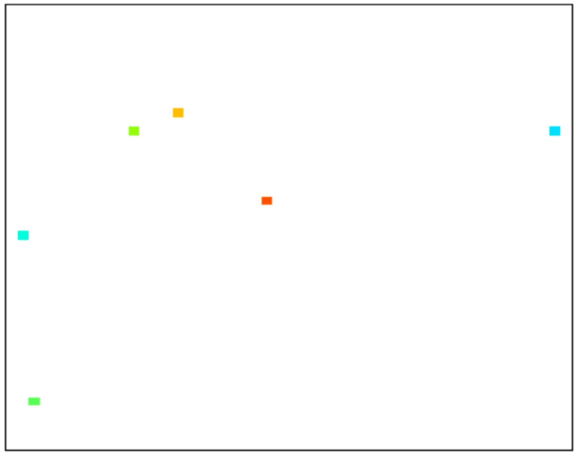
Example: 2000×2000 rank-8 random matrix

For illustration, we zoom in to a 50x50 submatrix

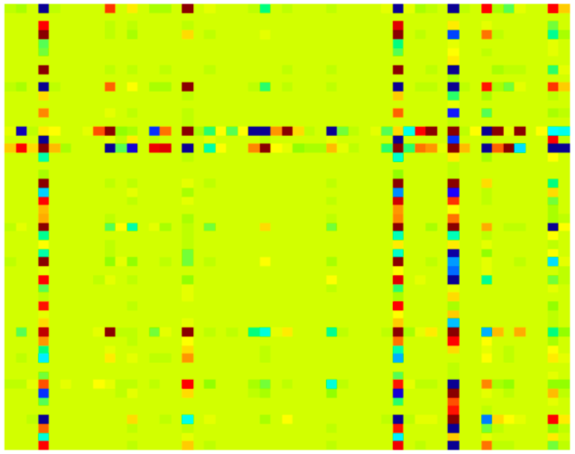
low-rank matrix $\mathbf{X}$



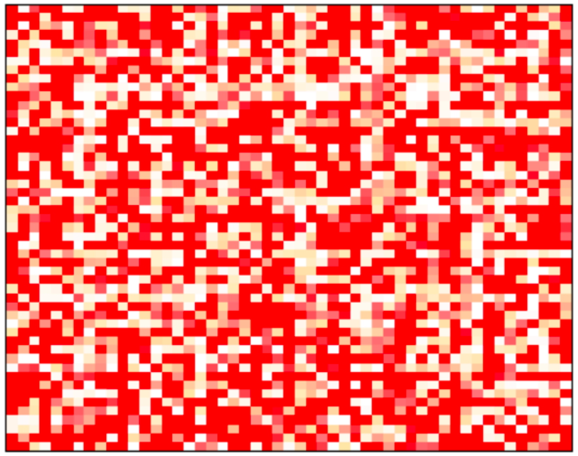
sampled matrix



Gradient descent output $\mathbf{UA}$



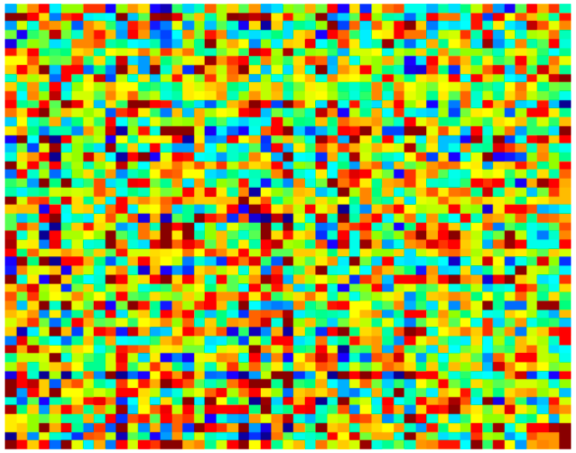
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



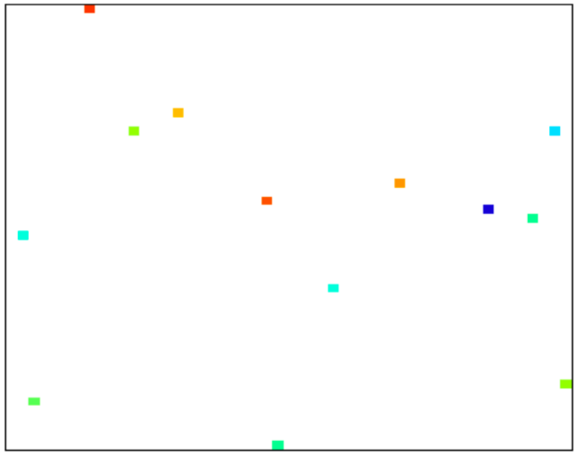
0.25% sampled

Example: 2000 $\times$ 2000 rank-8 random matrix

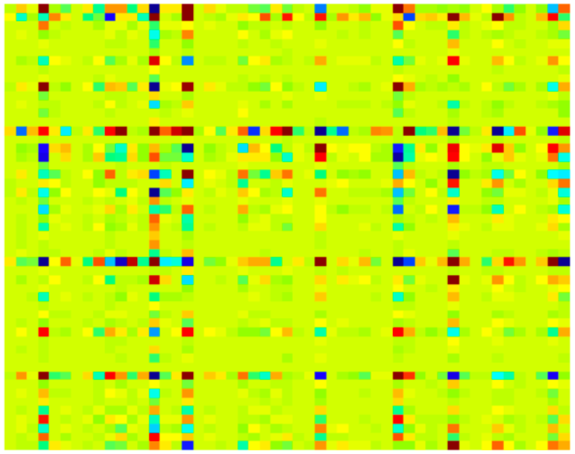
low-rank matrix $\mathbf{X}$



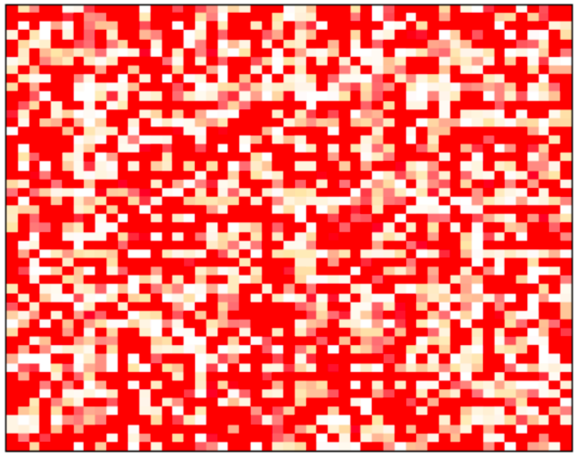
sampled matrix



Gradient descent output $\mathbf{UA}$



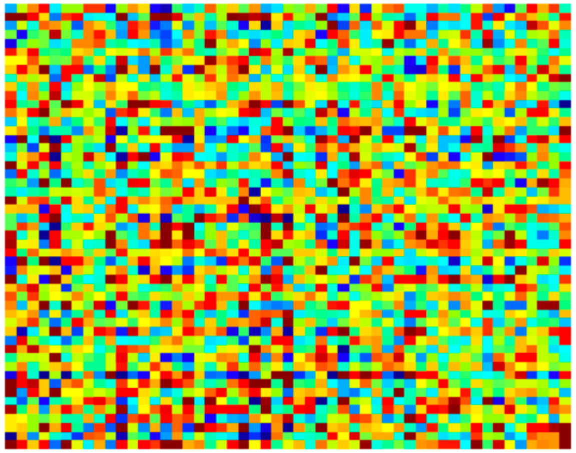
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



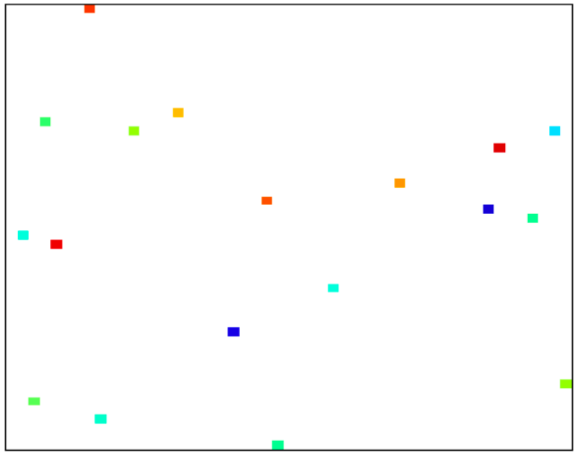
0.50% sampled

Example: 2000×2000 rank-8 random matrix

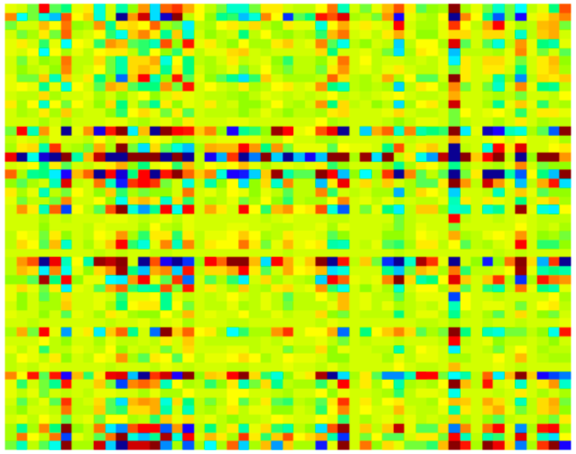
low-rank matrix $\mathbf{X}$



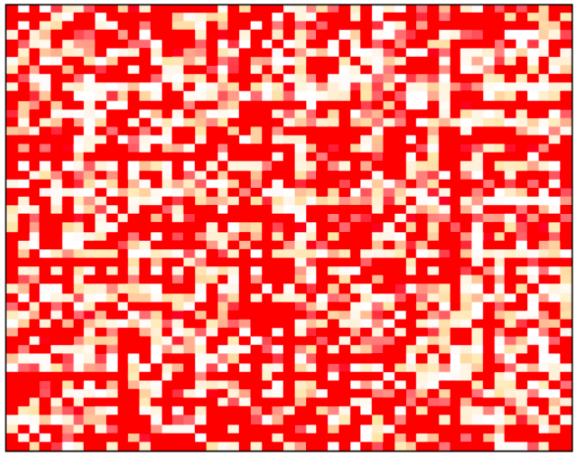
sampled matrix



Gradient descent output $\mathbf{UA}$



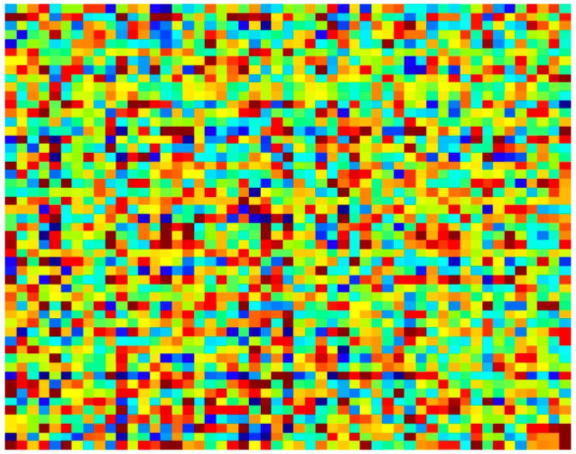
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



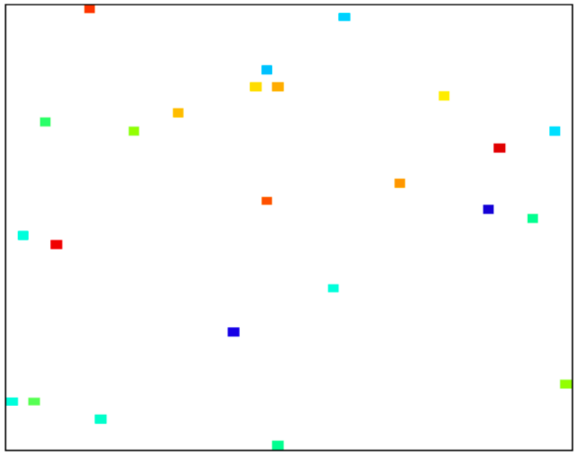
0.75% sampled

Example: 2000×2000 rank-8 random matrix

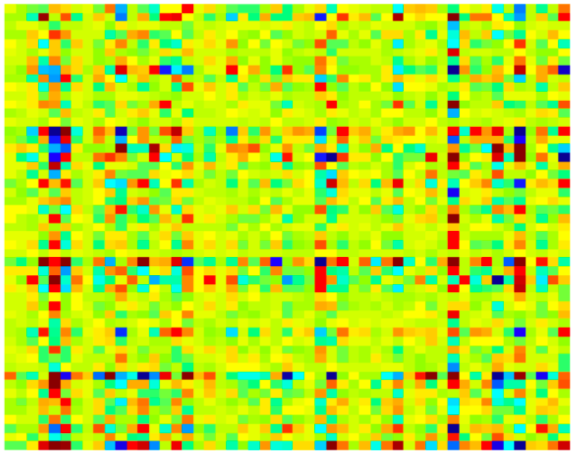
low-rank matrix $\mathbf{X}$



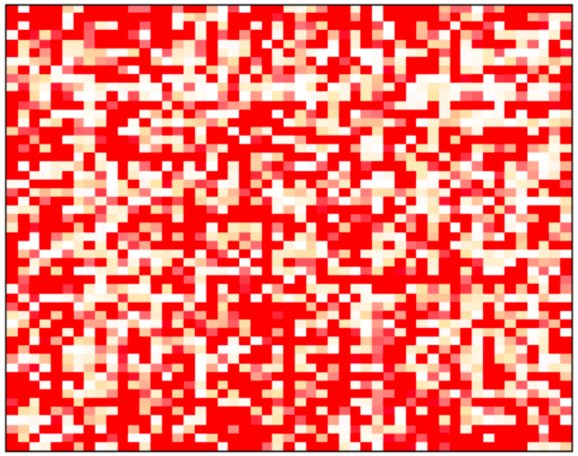
sampled matrix



Gradient descent output $\mathbf{UA}$



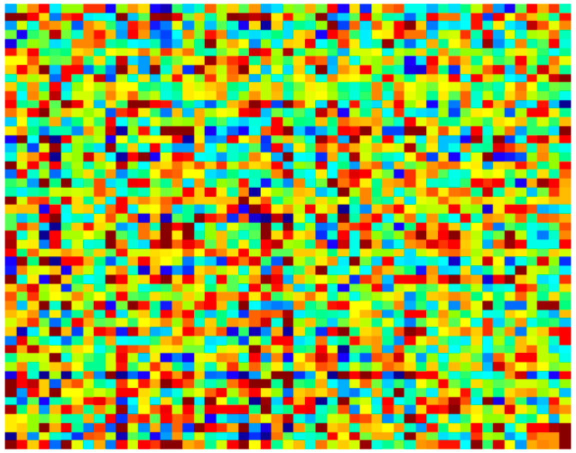
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



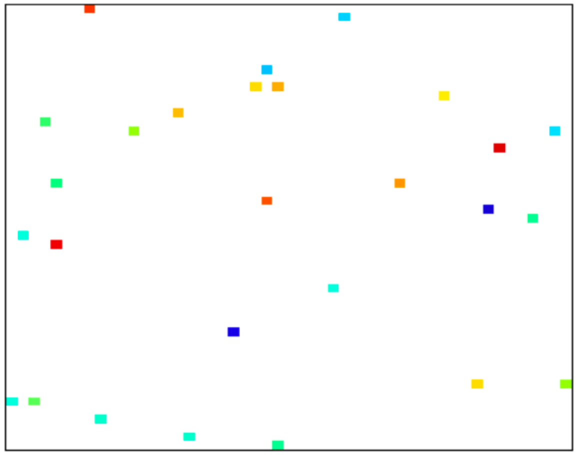
1.00% sampled

Example: 2000×2000 rank-8 random matrix

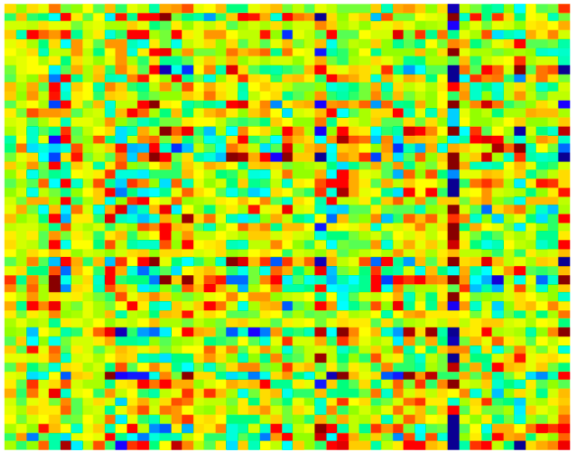
low-rank matrix $\mathbf{X}$



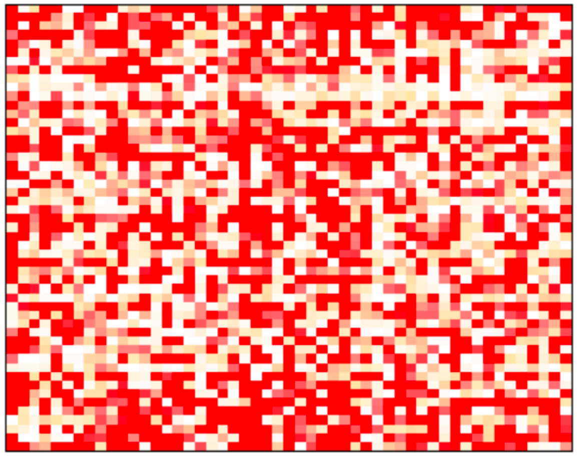
sampled matrix



Gradient descent output $\mathbf{UA}$



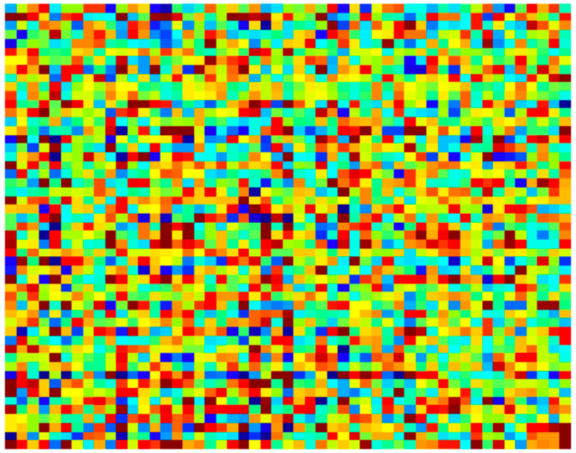
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



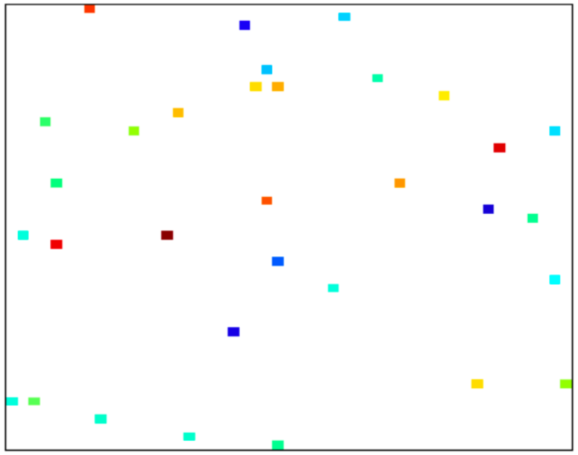
1.25% sampled

Example: 2000×2000 rank-8 random matrix

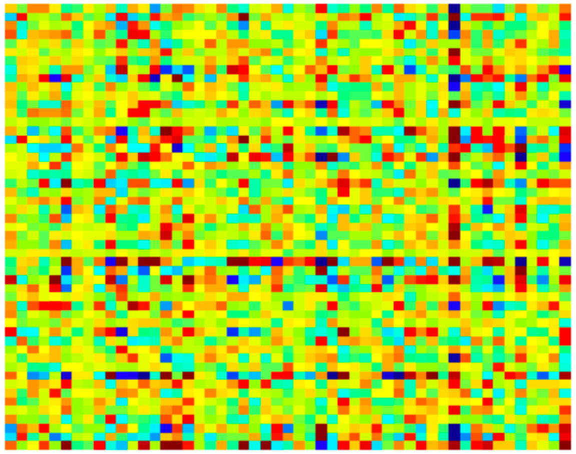
low-rank matrix $\mathbf{X}$



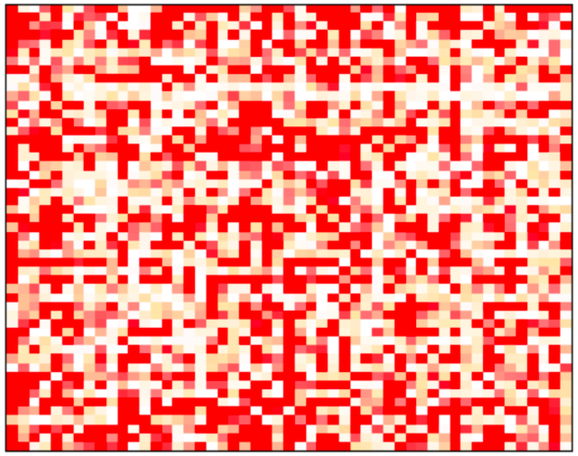
sampled matrix



Gradient descent output $\mathbf{UA}$



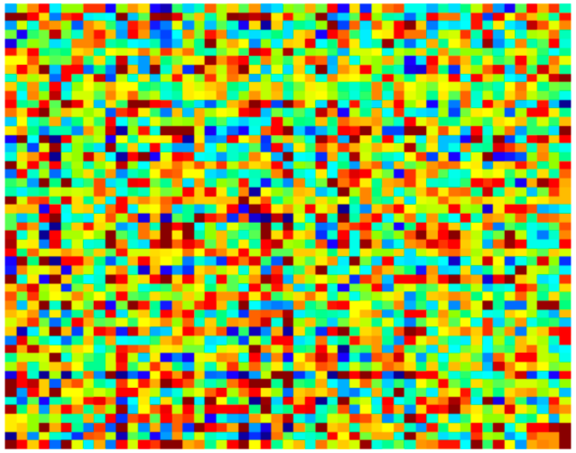
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



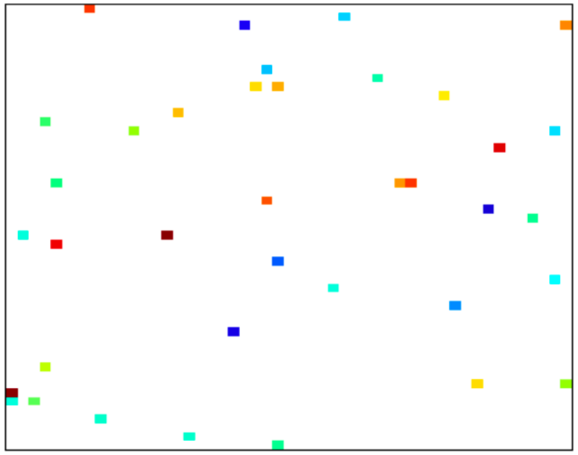
1.50% sampled

Example: 2000×2000 rank-8 random matrix

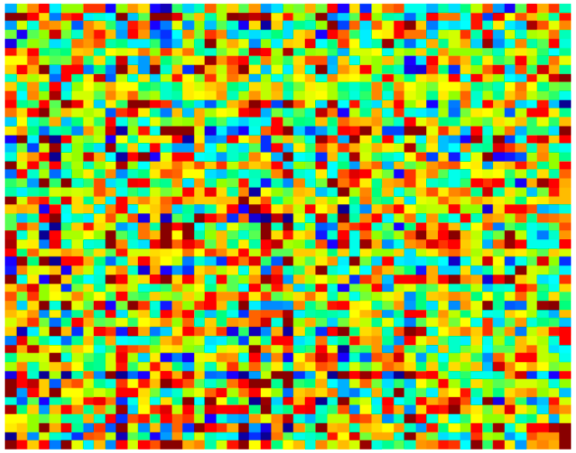
low-rank matrix $\mathbf{X}$



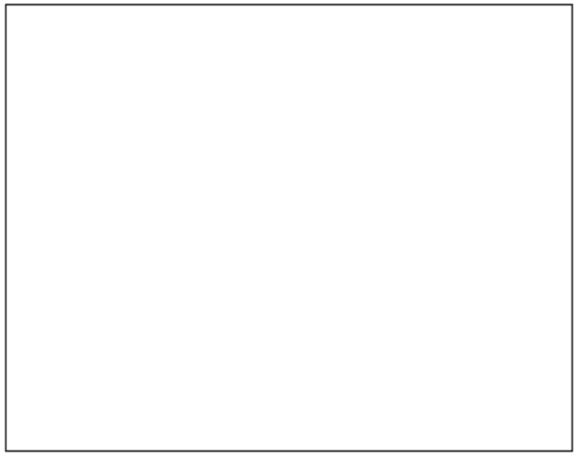
sampled matrix



Gradient descent output $\mathbf{UA}$



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



1.75% sampled

Matrix completion

- $$\text{minimize}_{\mathbf{U},\mathbf{A}} \sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} - v_j^T a_i)^2$$

- Gradient descent on $\{v_j\}_{j=1}^d$ and $\{a_i\}_{i=1}^n$ can be implemented via

$$v_j^{(t)} \leftarrow v_j^{(t-1)} - 2\eta \sum_{i\in S_j} ((v_j^{(t-1)})^T a_i^{(t-1)} - \mathbf{X}_{ji}) a_i^{(t-1)}$$

for all $j \in \{1,\ldots,d\}$, where S_j is the set of users who rated movie j and

$$a_i^{(t)} \leftarrow a_i^{(t-1)} - 2\eta \sum_{j\in S_i} ((v_j^{(t-1)})^T a_i^{(t-1)} - \mathbf{X}_{ji}) v_j^{(t-1)}$$

for all $i \in \{1,\ldots,n\}$, where S_i is the set of movies that were rated by user i

Matrix completion

- $$\text{minimize}_{\mathbf{U},\mathbf{A}} \sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} - v_j^T a_i)^2$$
- alternating minimization
    - repeat
        - fix v_j's and find optimal $a_i's$
            - for each i, set the gradient to zero: $2\sum_{j\in S_i} ((v_j^{(t-1)})^T a_i - \mathbf{X}_{ji})v_j^{(t-1)} \;=\; 0$, which gives

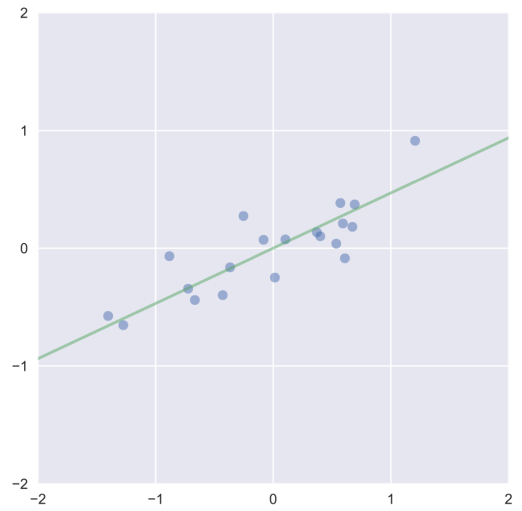
$$a_i\Big(\sum_{j\in S_i} v_j v_j^T\Big) = \sum_{j\in S_i} \mathbf{X_{ij}} v_j$$

$$a_i \;=\; \Big(\sum_{j\in S_i} v_j v_j^T\Big)^{-1} \sum_{j\in S_i} \mathbf{X_{ij}} v_j$$

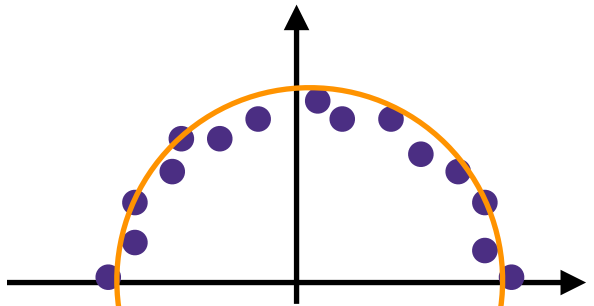
        - fix $a_i's$ and find optimal v_j's (similarly)

Autoencoders

- PCA is great in capturing variations in linear subspaces
    - It finds the best linear subspace for dimensionality reduction

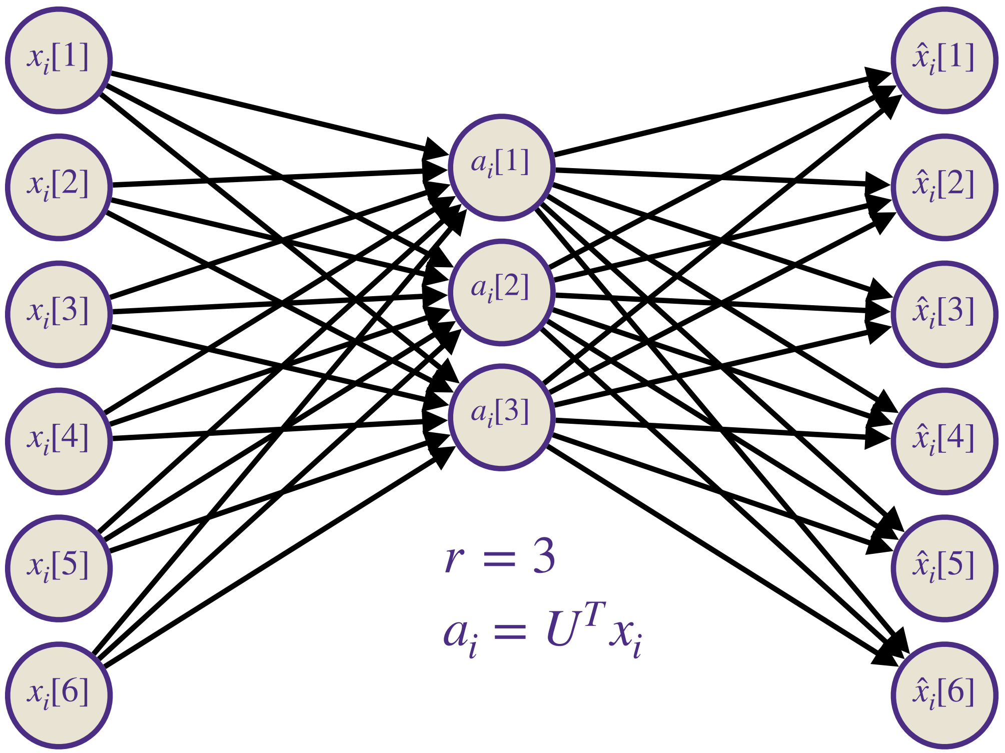


- PCA fails when variation is in non-linear manifolds
    - A non-linear encoding of data x_i for dimensionality reduction for these examples is to store the slope $\alpha_i = x_i[1]/x_i[2]$



Autoencoders

- Neural network perspective of PCA
  - Recall PCA reconstruction is $\hat{x}_i = UU^T x_i$, which can be encoded as a neural networks as follows
  - This is a special neural network for unsupervised learning (or label is the same as input), with first layer weight $U^T \in \mathbb{R}^{r\times d}$ with no activation function and second layer weight $U \in \mathbb{R}^{r\times d}$



$r = 3$

$a_i = U^T x_i$

$d = 6$

and data is centered

Output has the same dimension

$d = 6$

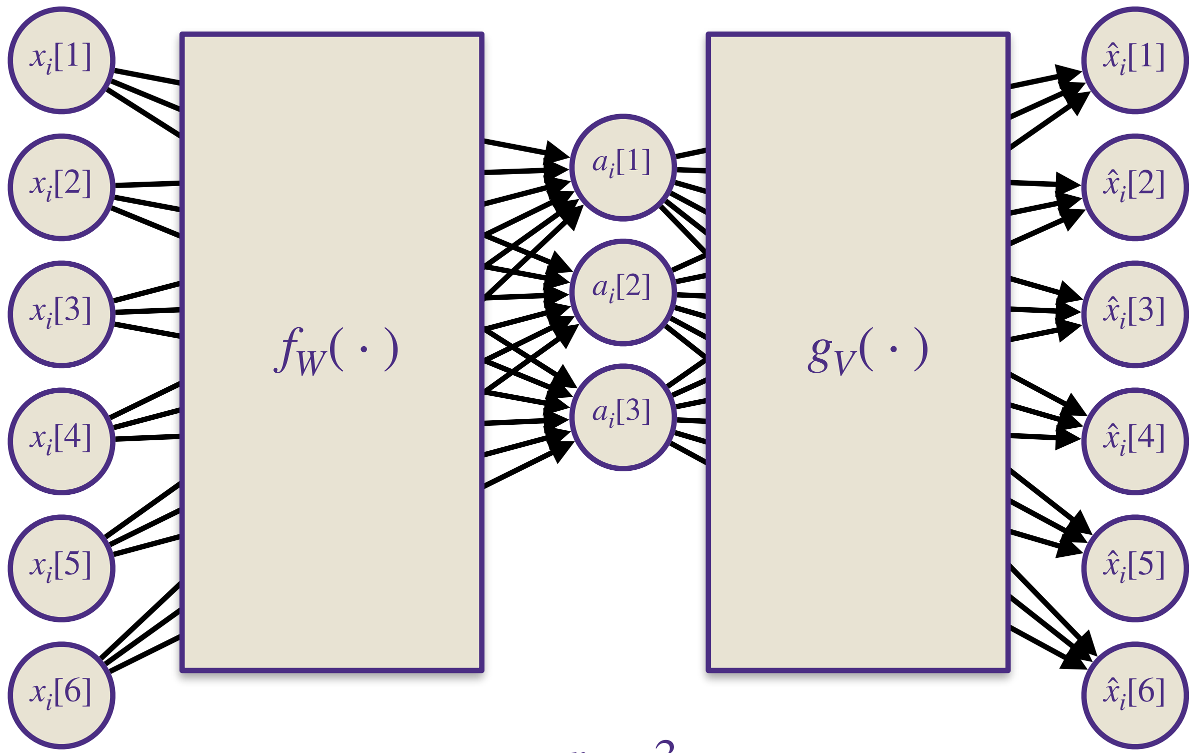
- We train the weights of this neural network to minimize the squared loss

$$\arg\min_U \sum_{i=1}^{n} \|x_i - \hat{x}_i\|_2^2$$

- PCA is the optimal solution of this neural network training

Autoencoders

- Autoencoders use neural networks to learn non-linear manifolds that minimize the reconstruction loss
  - $\hat{x}_i = g_V(f_W(x_i))$, where the encoder $f_W : \mathbb{R}^d \to \mathbb{R}^r$ and the decoder $g_V : \mathbb{R}^r \to \mathbb{R}^d$ are neural networks
  - We are essentially trying to learn the identity function, but with smaller (non-linear) dimensionality



- We train the weights of this neural network to minimize the squared loss

$$\arg\min_{U} \sum_{i=1}^{n} \|x_i - \hat{x}_i\|_2^2$$

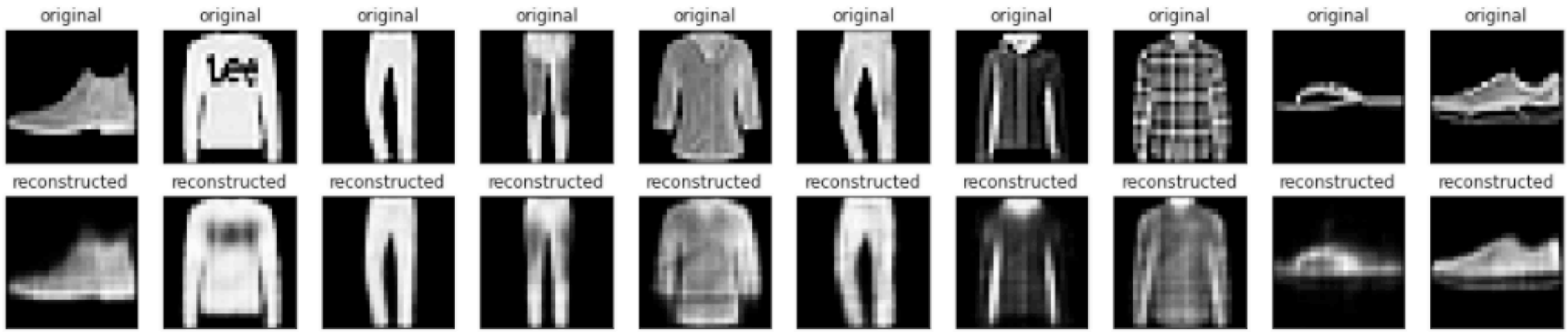
$d = 6$
and data is centered

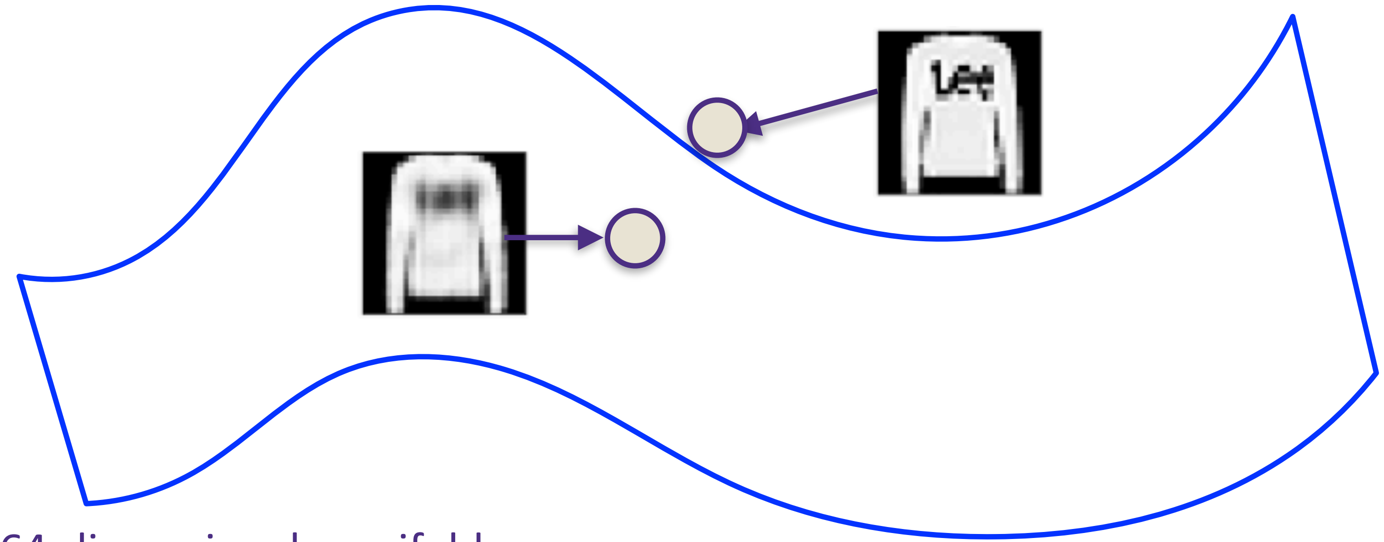
$r = 3$
$a_i = f_W(x_i)$

Output has the same dimension
$d = 6$

Example

- Autoencoder trained on Fashion MNIST dataset with r=64 and 2 fully connected layers for encoder and decoder

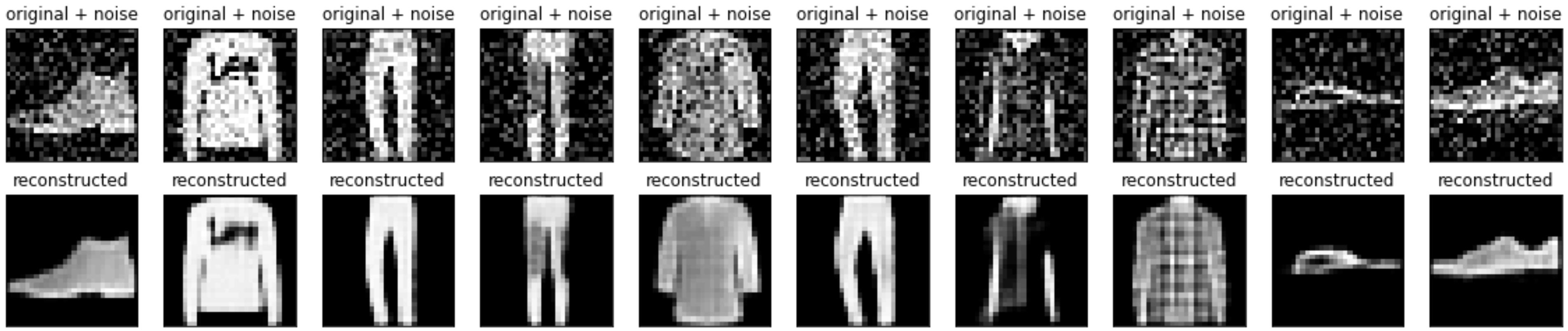


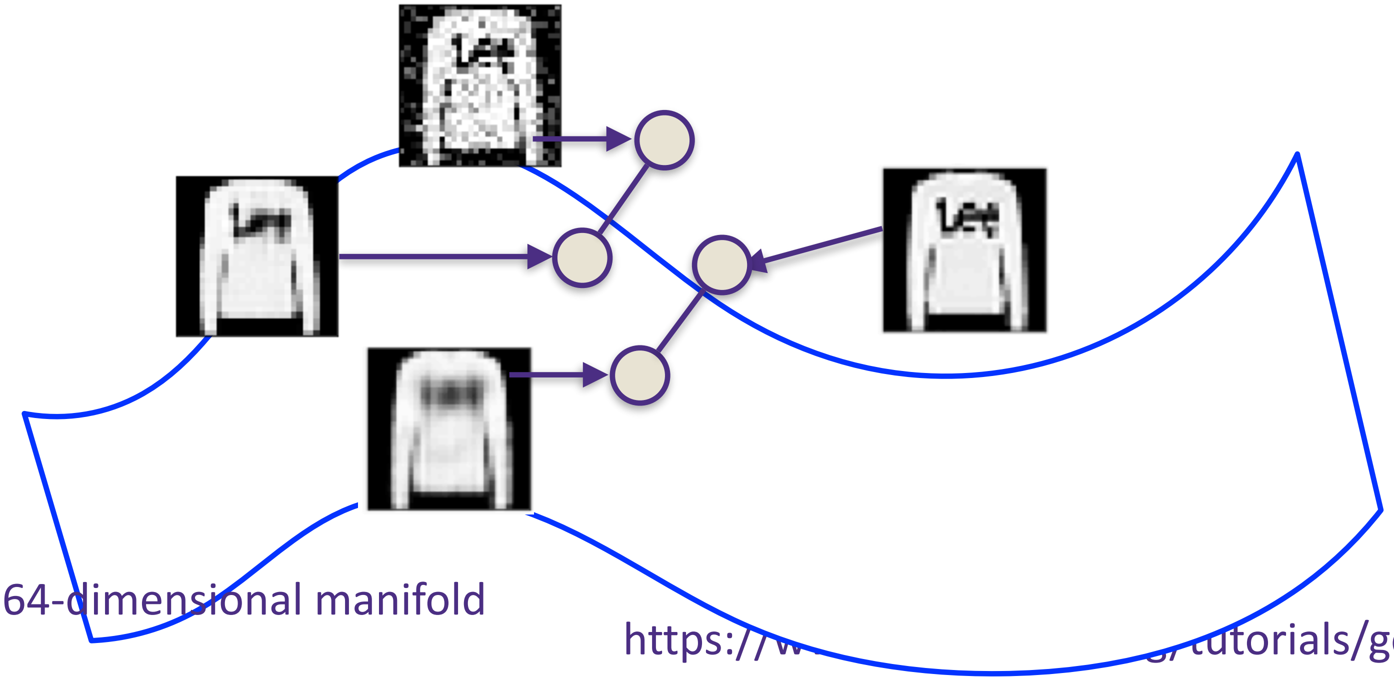


https://www.tensorflow.org/tutorials/generative/autoencoder

Example

- An autencoder trained on clean data can be used to denoise noisy data





https://w[illegible]g/tutorials/generative/autoencoder

Questions?

- Beyond obvious data compression and dimensionality reduction, such autoencoders have several important applications such as de-noising and anomaly detection

Lecture 24: Clustering with k-means

- Unsupervised learning
  - Dimensionality reduction
    - PCA
    - Auto-encoder
  - Clustering
    - **k-means**
    - Spectral,t-SNE,UMAP
  - Generative models
  - Density estimation

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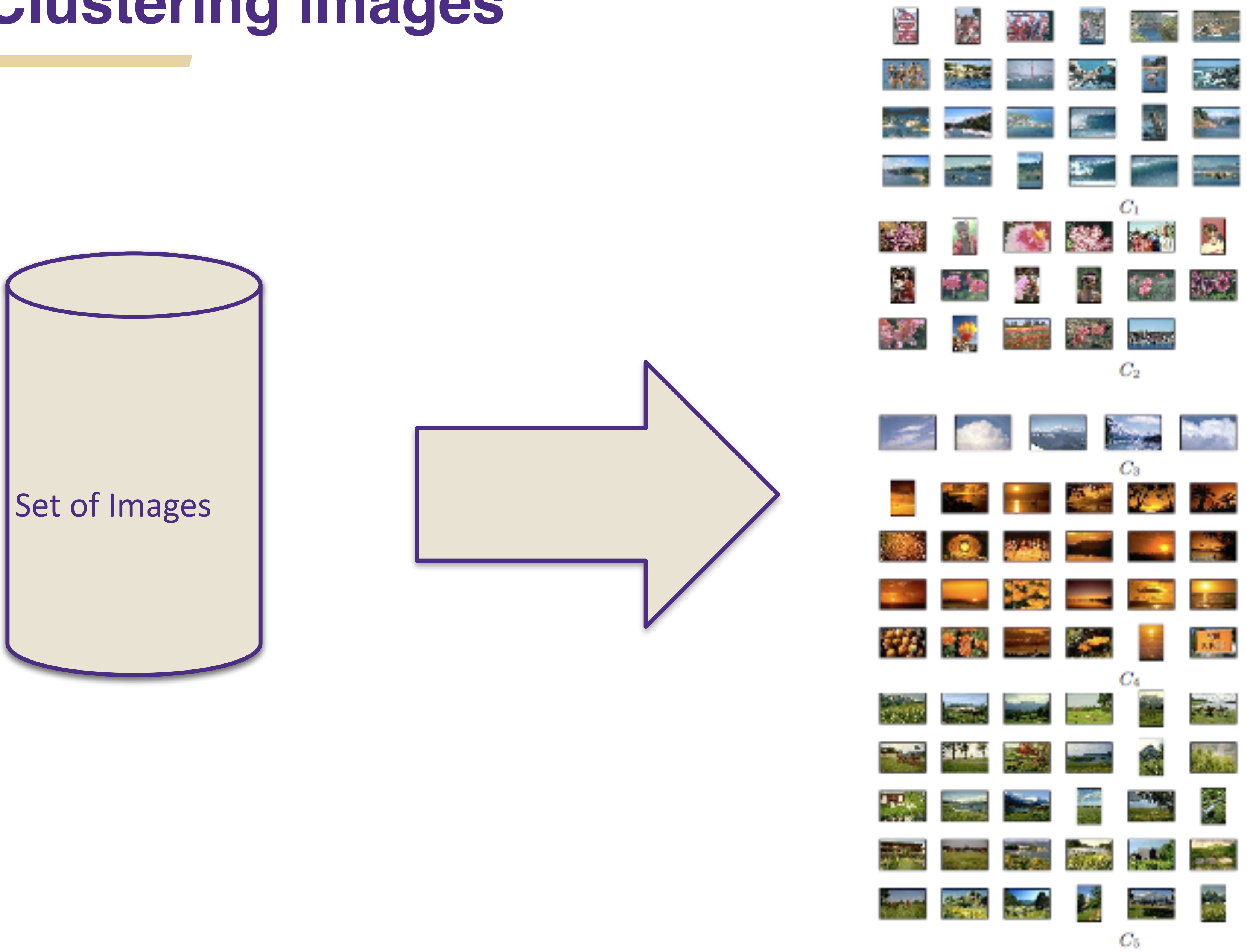
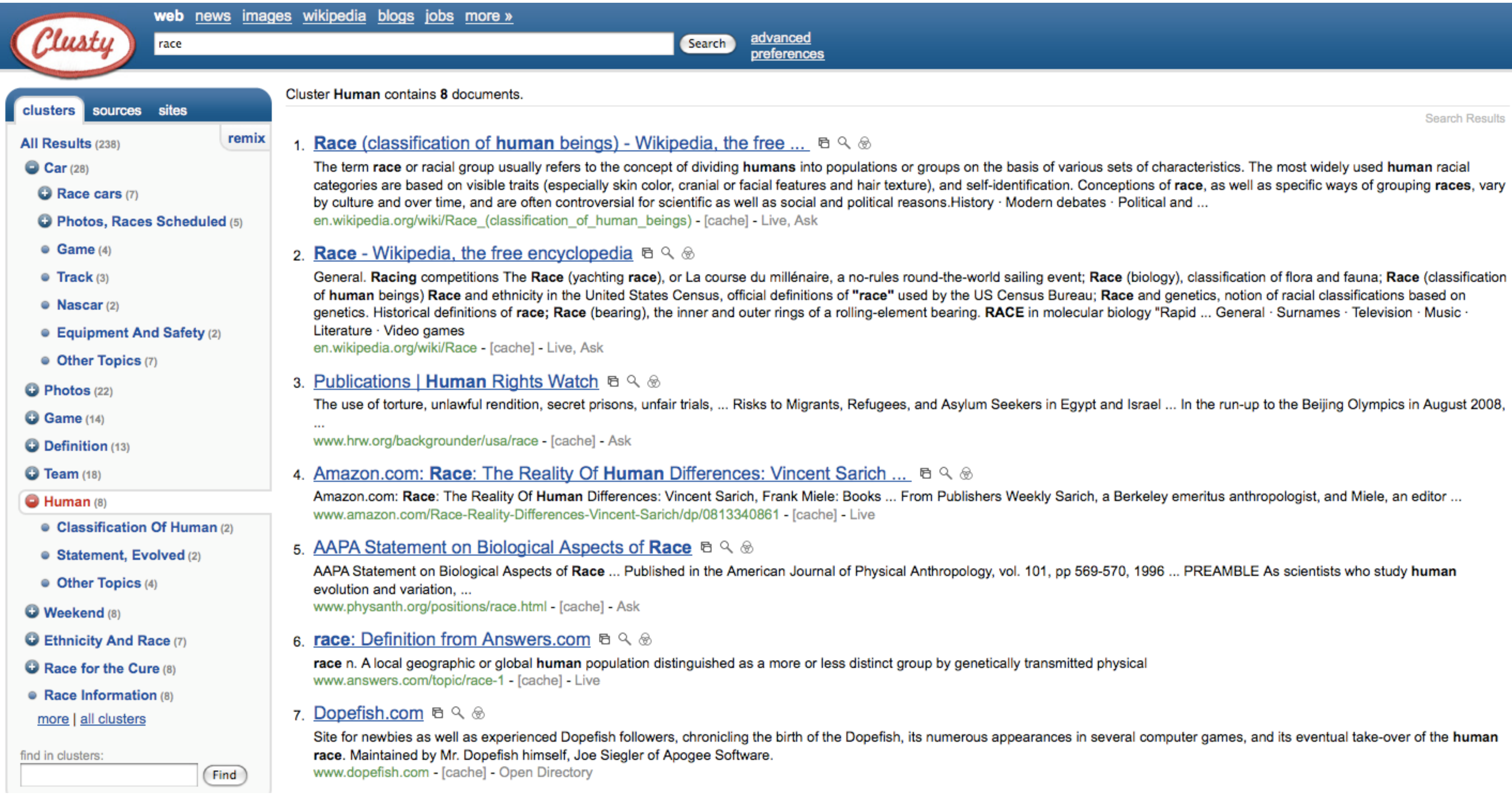
Clustering images



[Goldberger et al.]

Clustering web search results



All Results (238)
- Car (28)
  - Race cars (7)
  - Photos, Races Scheduled (5)
  - Game (4)
  - Track (3)
  - Nascar (2)
  - Equipment And Safety (2)
  - Other Topics (7)
- Photos (22)
- Game (14)
- Definition (13)
- Team (18)
- Human (8)
  - Classification Of Human (2)
  - Statement, Evolved (2)
  - Other Topics (4)
- Weekend (8)
- Ethnicity And Race (7)
- Race for the Cure (8)
- Race Information (8)

more | all clusters

find in clusters: Find

Cluster **Human** contains **8** documents.

Search Results

1. **Race** (classification of **human** beings) - Wikipedia, the free ...
   The term **race** or racial group usually refers to the concept of dividing **humans** into populations or groups on the basis of various sets of characteristics. The most widely used **human** racial categories are based on visible traits (especially skin color, cranial or facial features and hair texture), and self-identification. Conceptions of **race**, as well as specific ways of grouping **races**, vary by culture and over time, and are often controversial for scientific as well as social and political reasons.History · Modern debates · Political and ...
   en.wikipedia.org/wiki/Race_(classification_of_human_beings) - [cache] - Live, Ask

2. **Race** - Wikipedia, the free encyclopedia
   General. **Racing** competitions The **Race** (yachting **race**), or La course du millénaire, a no-rules round-the-world sailing event; **Race** (biology), classification of flora and fauna; **Race** (classification of **human** beings) **Race** and ethnicity in the United States Census, official definitions of **"race"** used by the US Census Bureau; **Race** and genetics, notion of racial classifications based on genetics. Historical definitions of **race; Race** (bearing), the inner and outer rings of a rolling-element bearing. **RACE** in molecular biology "Rapid ... General · Surnames · Television · Music · Literature · Video games
   en.wikipedia.org/wiki/Race - [cache] - Live, Ask

3. Publications | **Human** Rights Watch
   The use of torture, unlawful rendition, secret prisons, unfair trials, ... Risks to Migrants, Refugees, and Asylum Seekers in Egypt and Israel ... In the run-up to the Beijing Olympics in August 2008, ...
   www.hrw.org/backgrounder/usa/race - [cache] - Ask

4. Amazon.com: **Race**: The Reality Of **Human** Differences: Vincent Sarich ...
   Amazon.com: **Race**: The Reality Of **Human** Differences: Vincent Sarich, Frank Miele: Books ... From Publishers Weekly Sarich, a Berkeley emeritus anthropologist, and Miele, an editor ...
   www.amazon.com/Race-Reality-Differences-Vincent-Sarich/dp/0813340861 - [cache] - Live

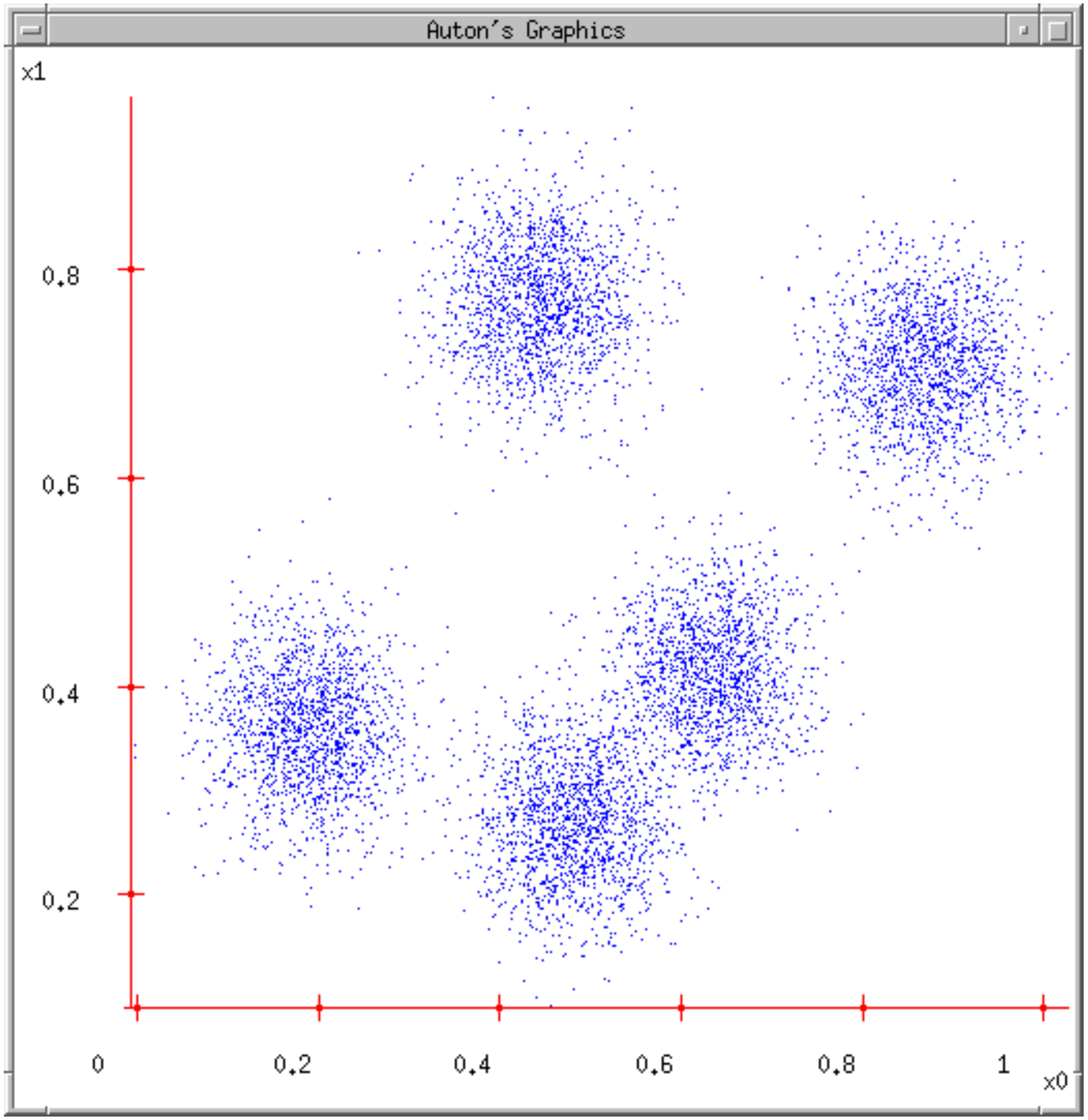
5. AAPA Statement on Biological Aspects of **Race**
   AAPA Statement on Biological Aspects of **Race** ... Published in the American Journal of Physical Anthropology, vol. 101, pp 569-570, 1996 ... PREAMBLE As scientists who study **human** evolution and variation, ...
   www.physanth.org/positions/race.html - [cache] - Ask

6. **race**: Definition from Answers.com
   race n. A local geographic or global **human** population distinguished as a more or less distinct group by genetically transmitted physical
   www.answers.com/topic/race-1 - [cache] - Live

7. Dopefish.com
   Site for newbies as well as experienced Dopefish followers, chronicling the birth of the Dopefish, its numerous appearances in several computer games, and its eventual take-over of the **human race**. Maintained by Mr. Dopefish himself, Joe Siegler of Apogee Software.
   www.dopefish.com - [cache] - Open Directory

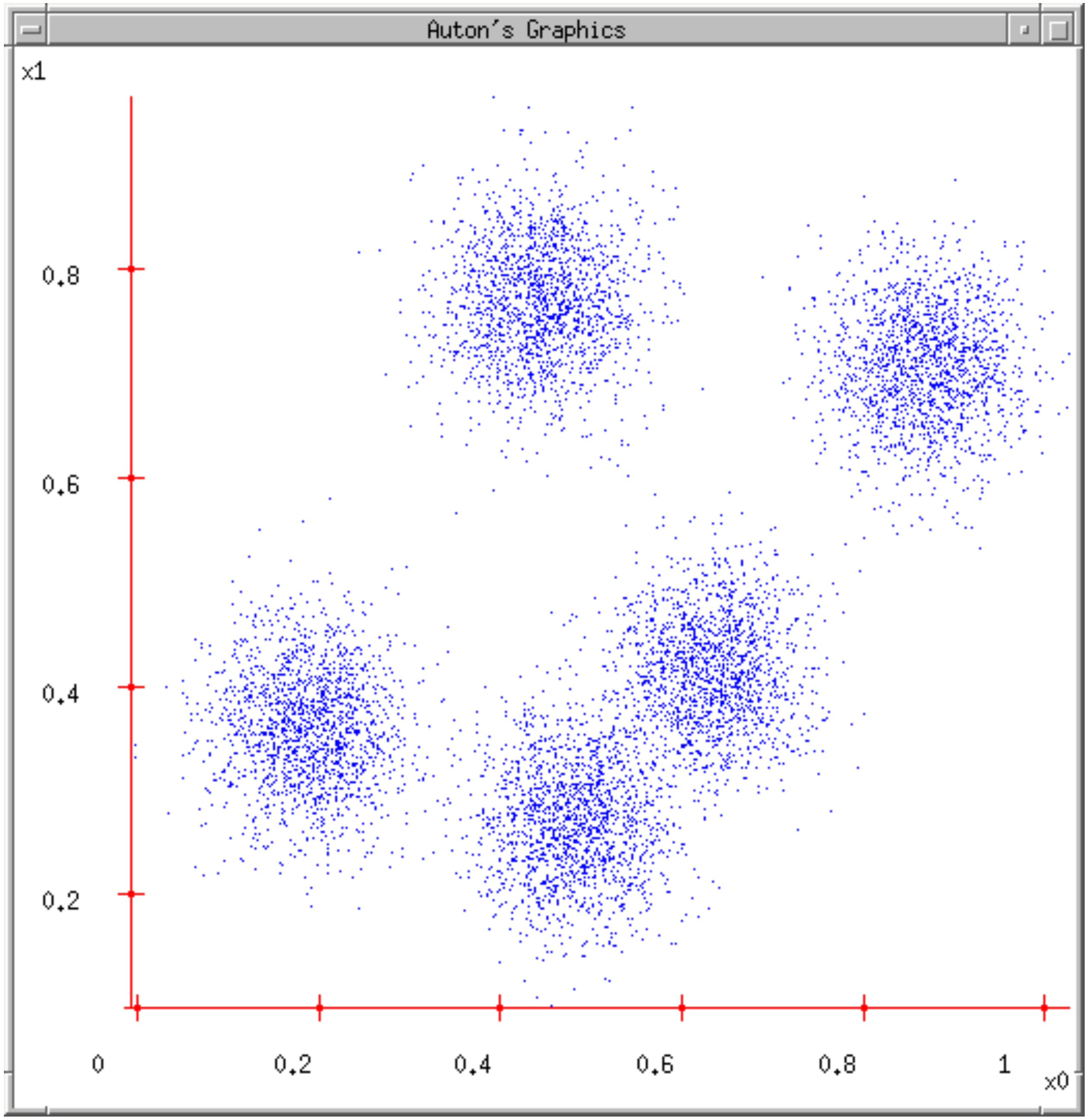
Some Data

- K-mean algorithm assumes this kind of structured data



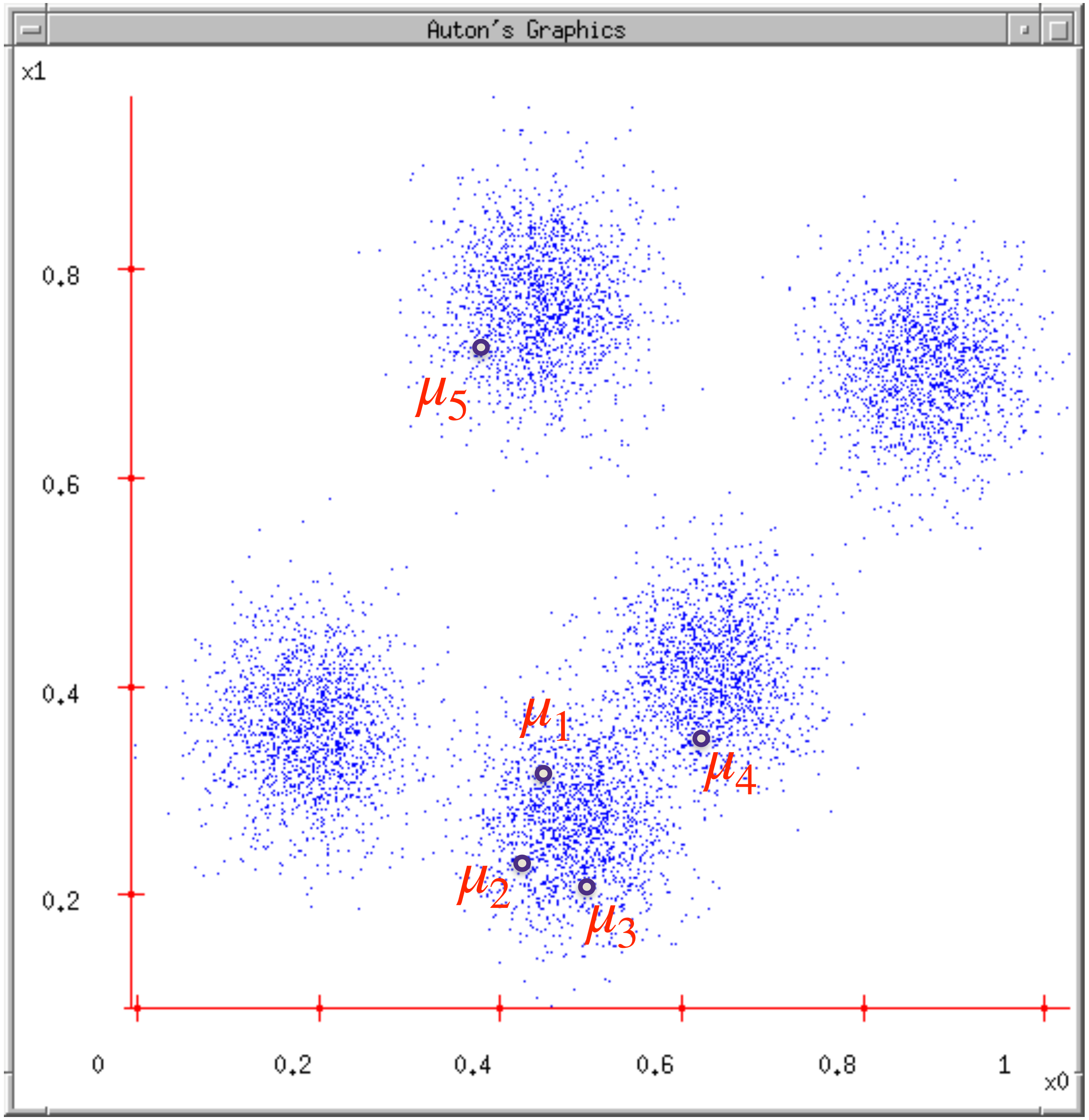
K-means

1. Ask user how many clusters they'd like. (e.g. k=5)



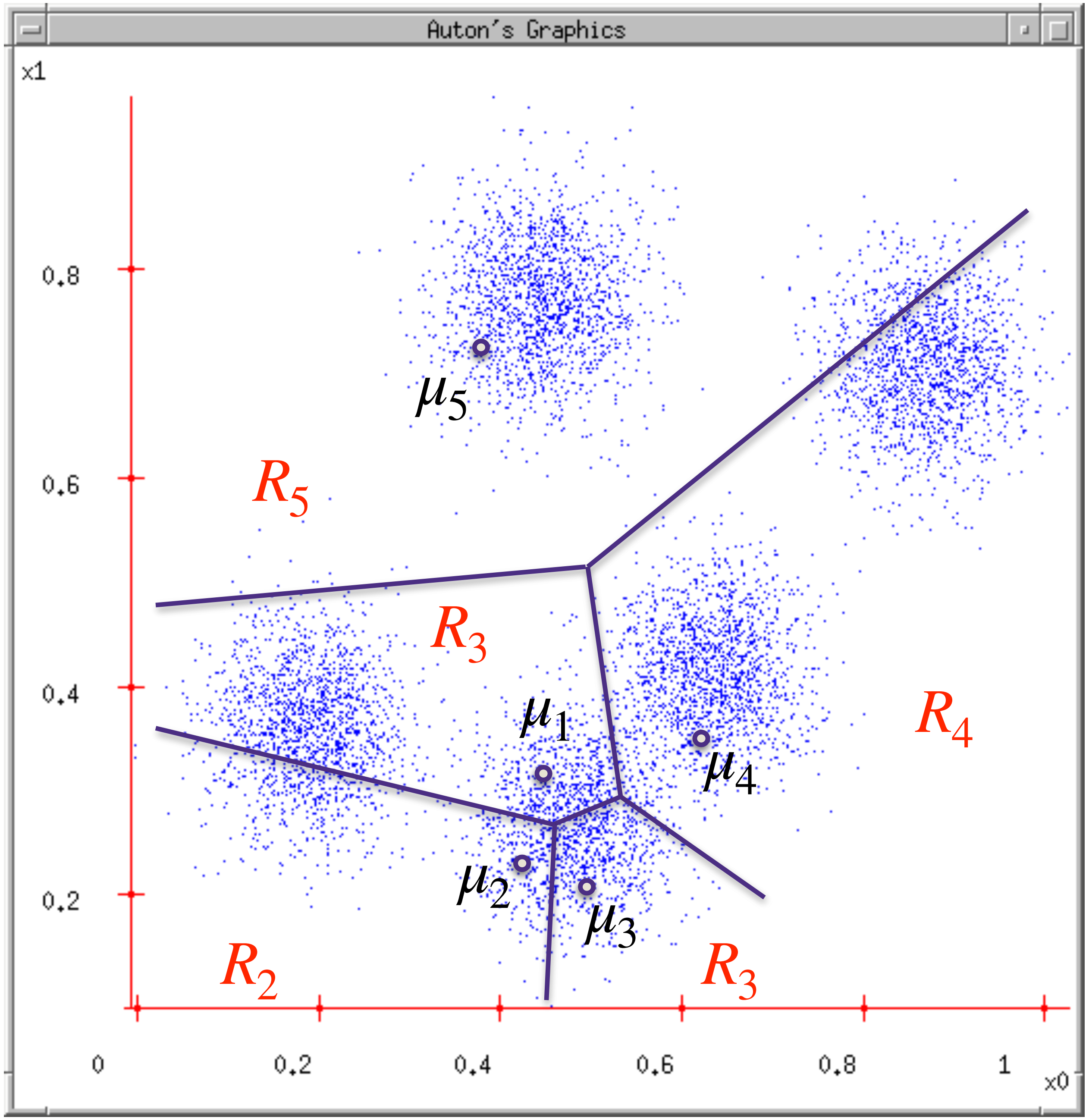
K-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations $\{\mu_1, \ldots, \mu_5\}$



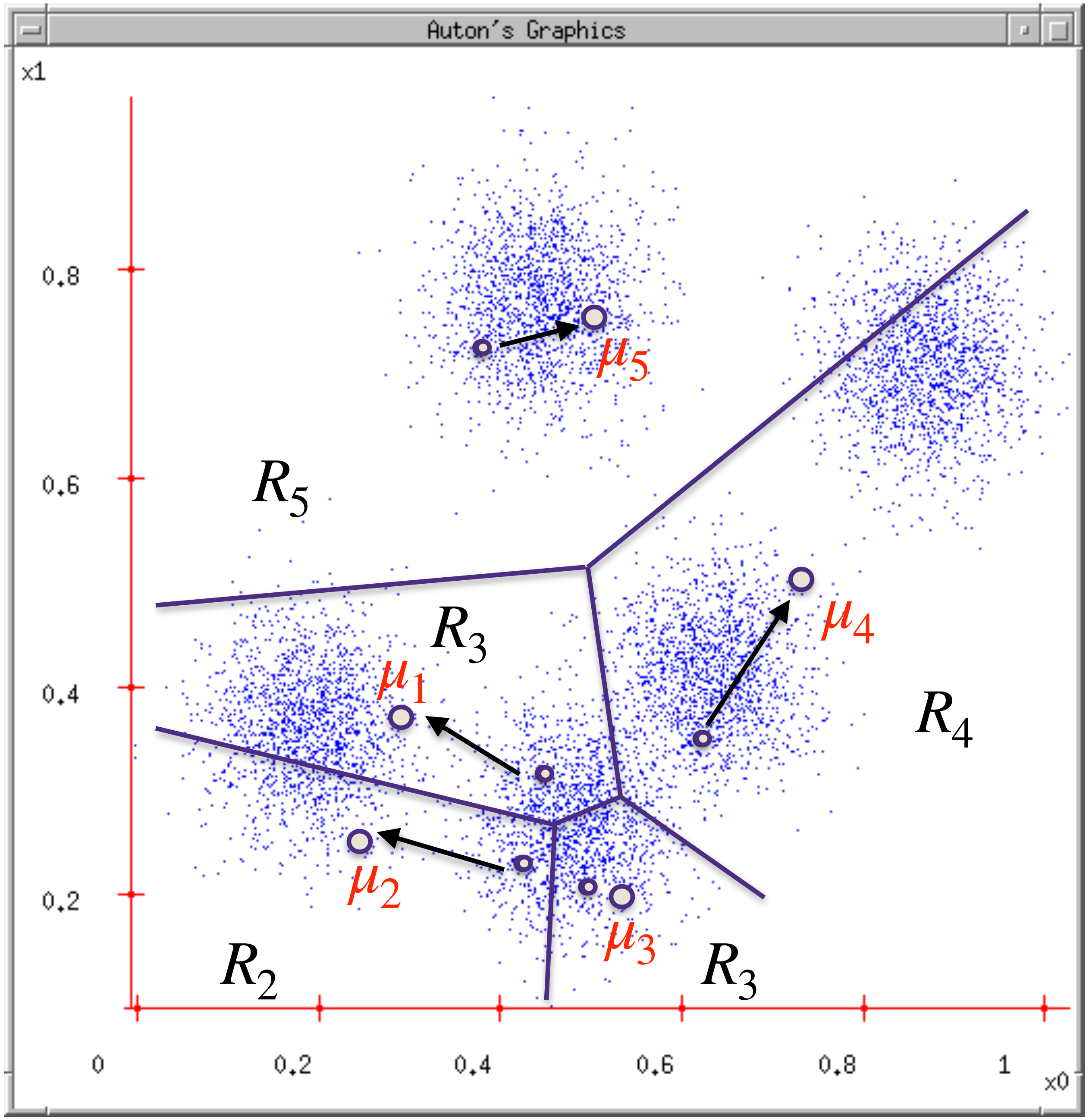
K-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations $\{\mu_1, \ldots, \mu_5\}$
3. Each datapoint finds out which Center it's closest to. (Thus each Center "owns" a set of datapoints)



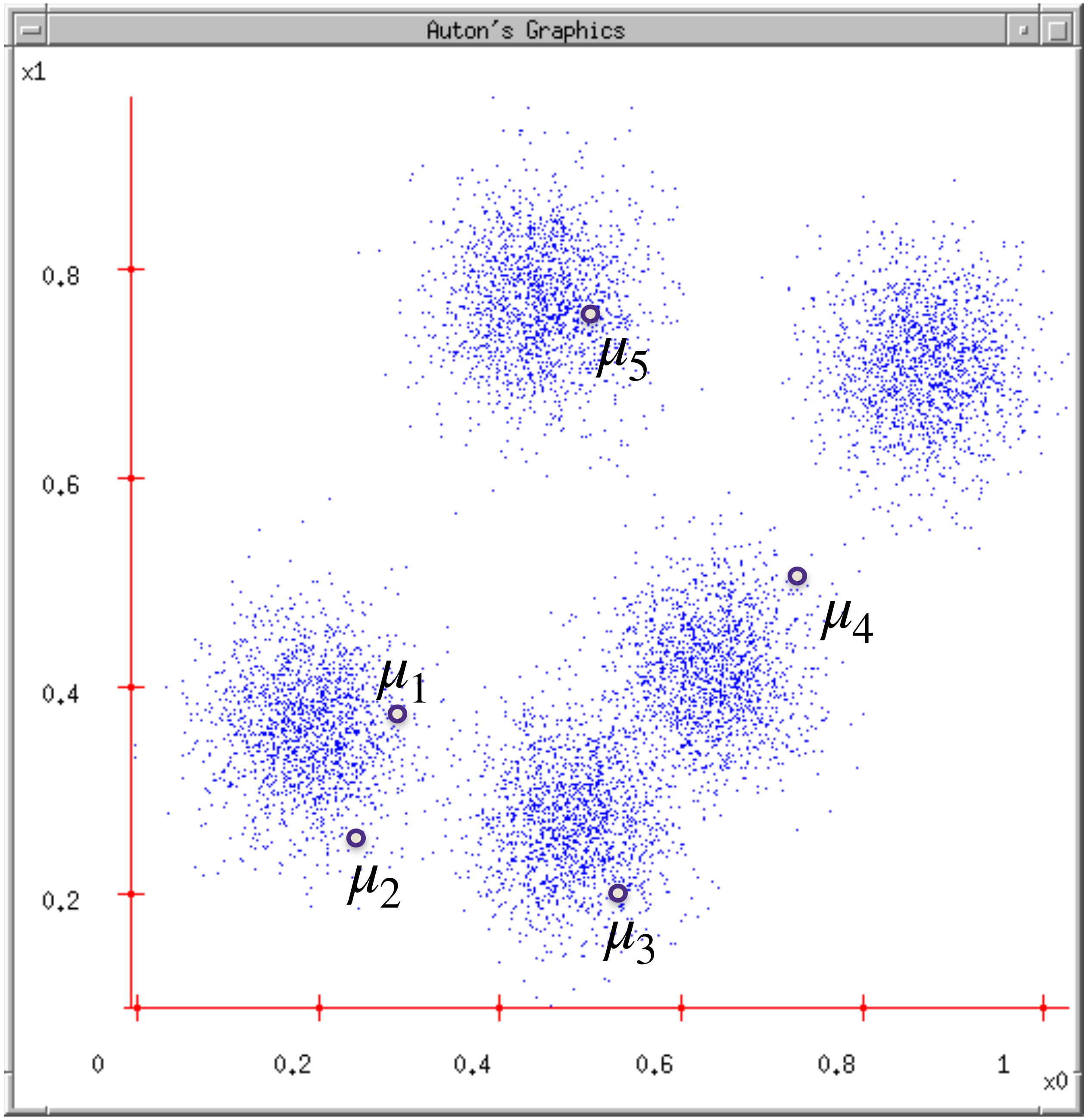
K-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations $\{\mu_1, \ldots, \mu_5\}$
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the centroid of the points it owns



K-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations $\{\mu_1, \ldots, \mu_5\}$
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the centroid of the points it owns…
5. …and jumps there
6. …Repeat until terminated!



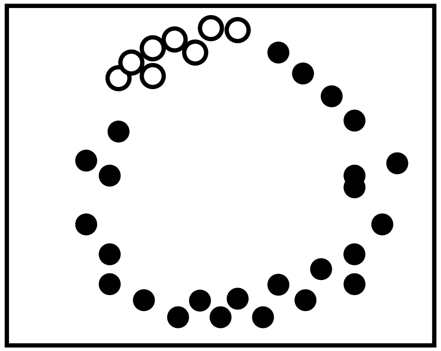
K-means

- Randomly initialize k centers
  - $\mu(0) = \mu_1(0), \ldots, \mu_k(0)$
- Classify: Assign each point j∈{1,…N} to nearest center:
  - Assignment: $C^{(t)}(j) \leftarrow \arg\min_i ||\mu_i - x_j||^2$
- Recenter: μ_i becomes centroid of its point:
  - $$\mu_i^{(t+1)} \leftarrow \arg\min_{\mu} \sum_{j:C(j)=i} ||\mu - x_j||^2$$
  - Equivalent to $\mu_i \leftarrow$ average of all the points assigned to μ_i!

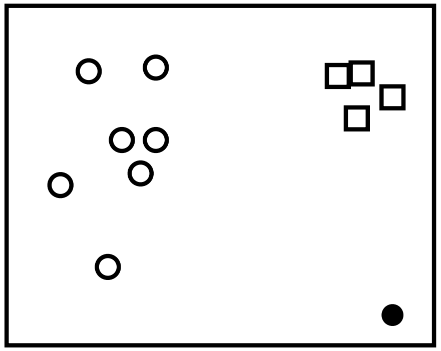
Which one is a snapshot of a converged k-means

When k-means is converged, there should be a set of centers and assignments that do not change when applying 1 step of k-means

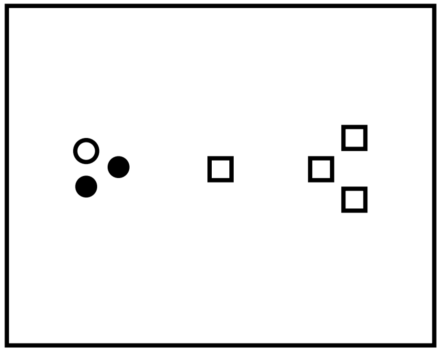
Example (a)



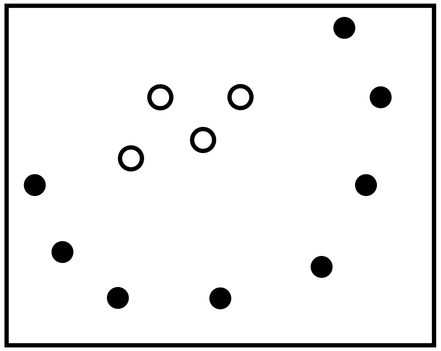
Example (b)



Example (c)



Example (d)



Does k-means converge??

- k-means is trying to minimize the following objective
- Optimize potential function:

$$\min_{\mu} \min_{C} F(\mu, C) = \min_{\mu} \min_{C} \sum_{i=1}^{k} \sum_{j:C(j)=i} ||\mu_i - x_j||^2$$

- Via alternating minimization
  - Fix μ, optimize C
  - Fix C optimize μ

Does k-means converge??

- there is only a finite set of values that $\{C(j)\}_{j=1}^n$ can take (k^n is large but finite)
- so there is only finite, k^n at most, values for cluster-centers also
- each time we update them, we will never increase the objective function $\sum_{i=1}^{k} \sum_{j:C(j)=i} \|x_j - \mu_i\|_2^2$
- the objective is lower bounded by zero
- after at most k^n steps, the algorithm must converge (as the assignments $\{C(j)\}_{j=1}^n$ cannot return to previous assignments in the course of k-means iterations)

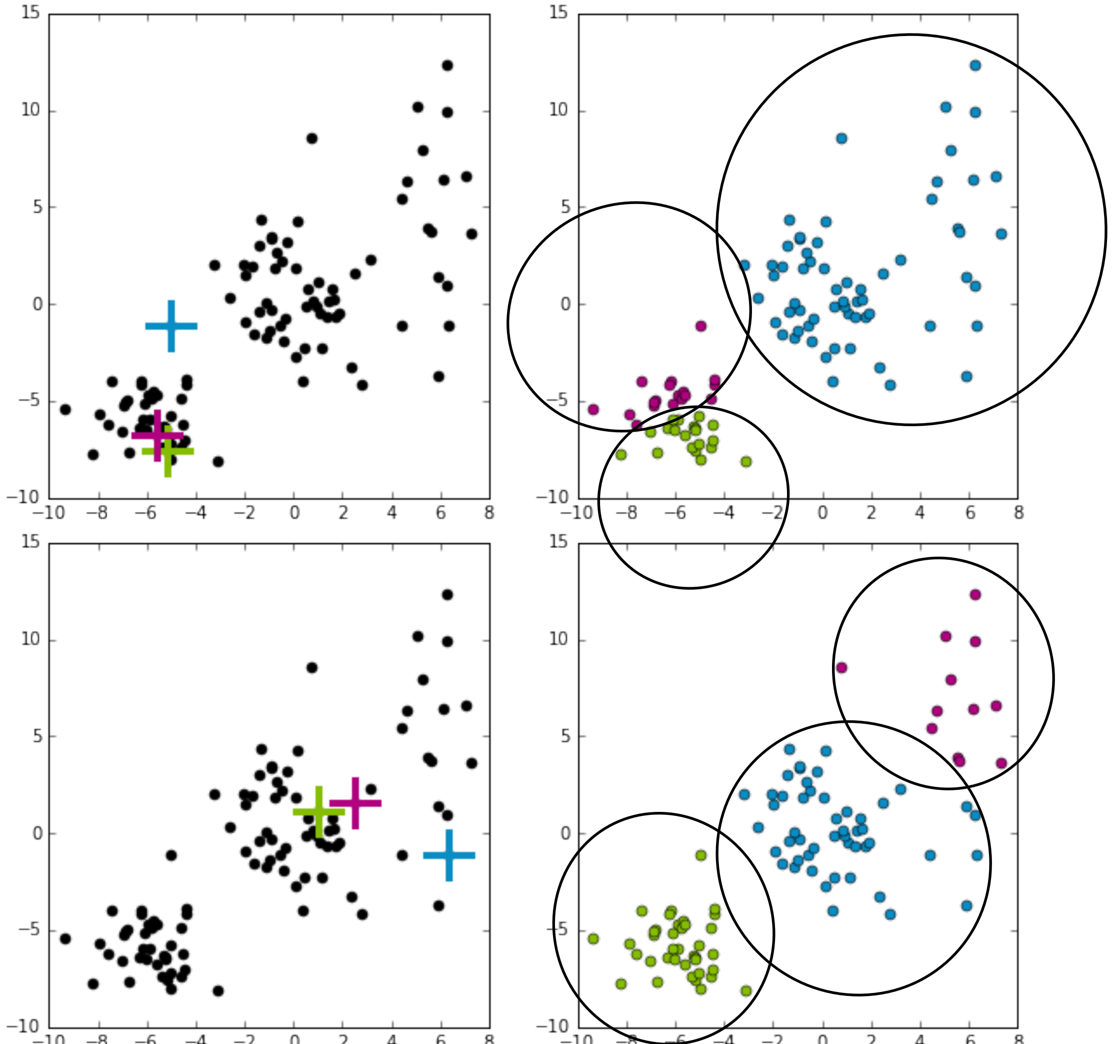
downsides of k-means

1. it requires the number of clusters K to be specified by us
2. the final solution depends on the initialization (does not find global minimum of the objective)

Initial position of centers final converged assignment

Trial 1

Trial 2



k-means++: a smart initialization

Smart initialization:

1. Choose **first** cluster center uniformly at random from data points

2. Repeat ***K-1*** times

    3. For each data point $\boldsymbol{x_i}$, compute distance $\boldsymbol{d_i}$ to nearest cluster center

    4. Choose new cluster center from amongst data points, with probability

of $\boldsymbol{x_i}$ being chosen proportional to $\boldsymbol{(d_i)^2}$

- apply standard K-means after the initialization

Questions?

Lecture 25:

- Unsupervised learning
    - Dimensionality reduction
        - PCA
        - Auto-encoder
    - Clustering
        - k-means
        - **Spectral,t-SNE,UMAP**
    - Generative models
    - Density estimation

Questions?

Questions?