Shameless plug for my course next quarter

CSE 599: Online and Adaptive Methods for Machine Learning.

Webpage: https://courses.cs.washington.edu/courses/cse599i/18wi/
Non-CSE need add-codes: https://goo.gl/forms/G76D6cOKNtdBlbe62

The standard approach to machine learning uses a training set of labeled examples to learn a prediction rule that will predict the labels of new examples. Collecting such training sets can be expensive and time-consuming. This course will explore methods that leverage already-collected data to guide future measurements, in a closed loop, to best serve the task at hand. We focus on two paradigms: i) in pure-exploration we desire algorithms that identify or learn a good model using as few measurements as possible (e.g., classification, drug discovery, science), and ii) in regret minimization we desire algorithms that balance taking measurements to learn a model with taking measurements to exploit the model to obtain high reward outcomes (e.g., medical treatment design, ad-serving). The course will assume introductory machine learning (e.g., CSE 546) and maturity in topics like linear algebra, statistics, and calculus. The course will be analysis heavy, with a focus on methods that work well in practice.

Practice

- Fill in the missing plots:

$$\Sigma = \mathbf{X}^T \mathbf{J}\mathbf{J}\mathbf{X} = \mathbf{Z}^T \mathbf{J}\mathbf{J}\mathbf{Z}$$

$$\mathbf{V}\mathbf{S}\mathbf{V}^T = \mathrm{eig}(\Sigma) \qquad \mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n$$

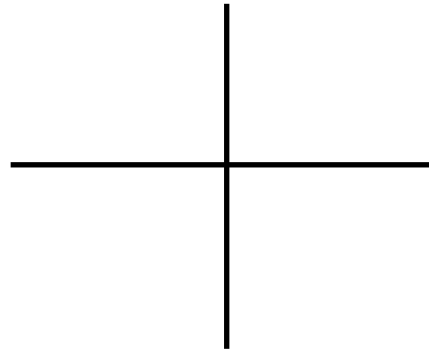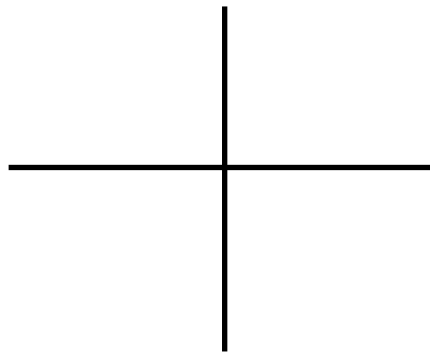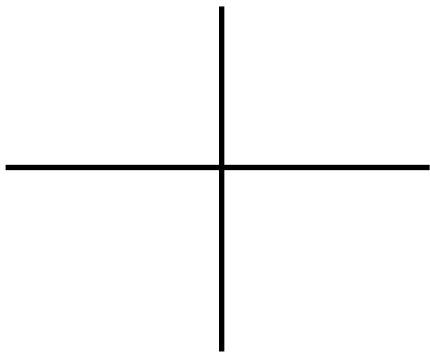$$\mu_X = \mathbf{X}^T \mathbf{1}/n \qquad \mu_Z = \mathbf{Z}^T \mathbf{1}/n$$

$$\mathbf{X} \qquad \mathbf{Z} \qquad\qquad \mu_X - \mu_Z \qquad \mathbf{V}S^{-1/2}\mathbf{V}^T(\mu_X - \mu_Z)$$

Principal Component Analysis (continued)

Machine Learning – CSE546

Kevin Jamieson

University of Washington

November 16, 2017

Linear projections

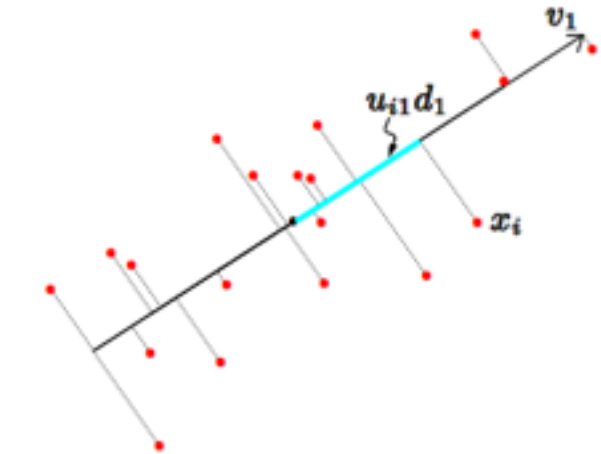Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} \|(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})\|^2.$$

where $\mathbf{V}_q = [v_1, v_2, \ldots, v_q]$ is orthonormal:

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

Principal Component Analysis (PCA) projects $(\mathbf{X} - \mathbf{1}\bar{x}^T)$ down onto $\mathbf{V}_q$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U}_q \text{diag}(d_1, \ldots, d_q) \qquad \mathbf{U}_q^T \mathbf{U}_q = I_q$$
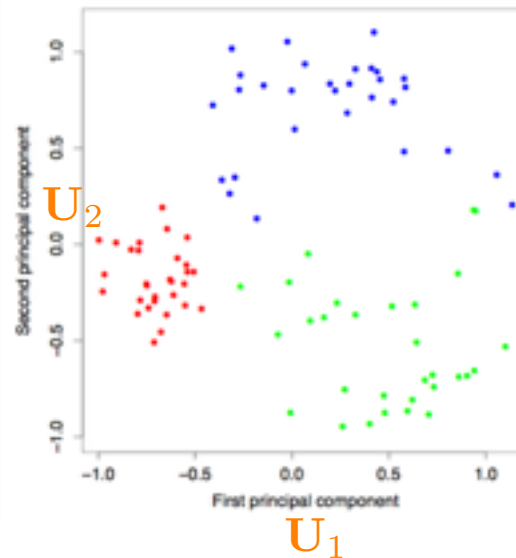
Singular Value Decomposition defined as

$$\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$$

Dimensionality reduction

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$
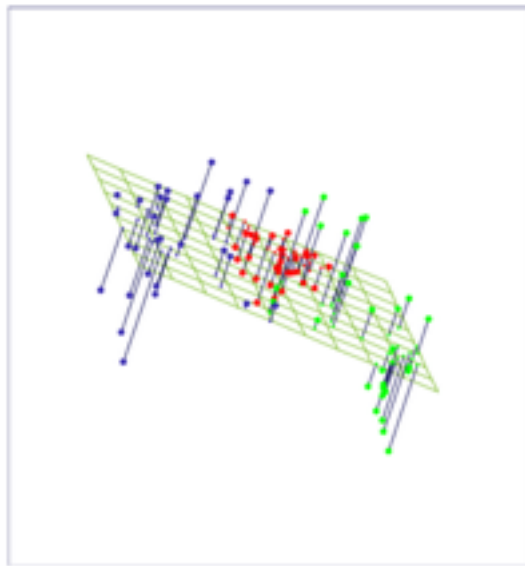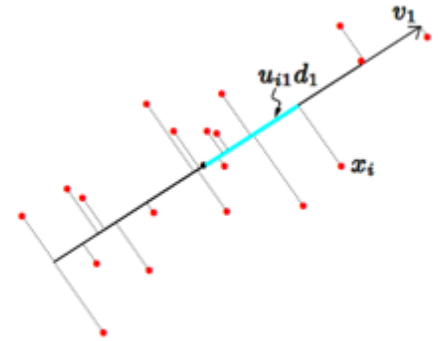

$$\mathbf{X} - \mathbf{1}\bar{x}^T$$

Power method - one at a time

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T \qquad v_* = \arg\max_v \; v^T \Sigma v$$

$$v_{k+1} = \frac{\Sigma v_k}{||\Sigma v_k||} \qquad\qquad v_0 \sim \mathcal{N}(0, I)$$

Matrix completion

Given historical data on how users rated movies in past:

NETFLIX

17,700 movies, 480,189 users, 99,072,112 ratings   (Sparsity: 1.2%)

Predict how the same users will rate movies in the future (for $1 million prize)

Alice	1	?	?	4	?
Bob	?	2	5	?	?
Carol	?	?	4	5	?
Dave	5	?	?	?	4

Matrix completion

n movies, m users, |S| ratings

$$\underset{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}}{\arg\min} \sum_{(i,j,s) \in \mathcal{S}} ||(UV^T)_{i,j} - s_{i,j}||_2^2$$

How do we solve it? With full information?

Matrix completion

n movies, m users, |S| ratings

$$\underset{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}}{\arg\min} \sum_{(i,j,s) \in \mathcal{S}} ||(UV^T)_{i,j} - s_{i,j}||_2^2$$

Random projections

PCA finds a low-dimensional representation that reduces population variance

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

$\mathbf{V}_q \mathbf{V}_q^T$ is a *projection matrix* that minimizes error in basis of size q

$\mathbf{V}_q$ are the first q eigenvectors of Σ

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

But what if I care about the reconstruction of the *individual* points?

$$\min_{\mathbf{W}_q} \max_{i=1,\ldots,n} ||(x_i - \bar{x}) - \mathbf{W}_q \mathbf{W}_q^T (x_i - \bar{x})||^2$$

Random projections

$$\min_{\mathbf{W}_q} \max_{i=1,\ldots,n} ||(x_i - \bar{x}) - \mathbf{W}_q \mathbf{W}_q^T (x_i - \bar{x})||^2$$

Johnson-Lindenstrauss (1983)

Theorem 1.1. *(Johnson-Lindenstrauss) Let $\epsilon \in (0, 1/2)$. Let $Q \subset \mathbb{R}^d$ be a set of n points and $k = \frac{20 \log n}{\epsilon^2}$. There exists a Lipshcitz mapping $f : \mathbb{R}^d \to \mathbb{R}^k$ such that for all $u, v \in Q$:* (independent of d)

$$(1 - \epsilon)\|u - v\|^2 \leq \|f(u) - f(v)\|^2 \leq (1 + \epsilon)\|u - v\|^2$$

Theorem 1.2. *(Norm preservation) Let $x \in \mathbb{R}^d$. Assume that the entries in $A \subset \mathbb{R}^{k \times d}$ are sampled independently from $N(0, 1)$. Then,*

$$\Pr((1 - \epsilon)\|x\|^2 \leq \|\frac{1}{\sqrt{k}} Ax\|^2 \leq (1 + \epsilon)\|x\|^2) \geq 1 - 2e^{-(\epsilon^2 - \epsilon^3)k/4}$$

Nonlinear dimensionality reduction

Find a low dimensional representation that respects "local distances" in the higher dimensional space
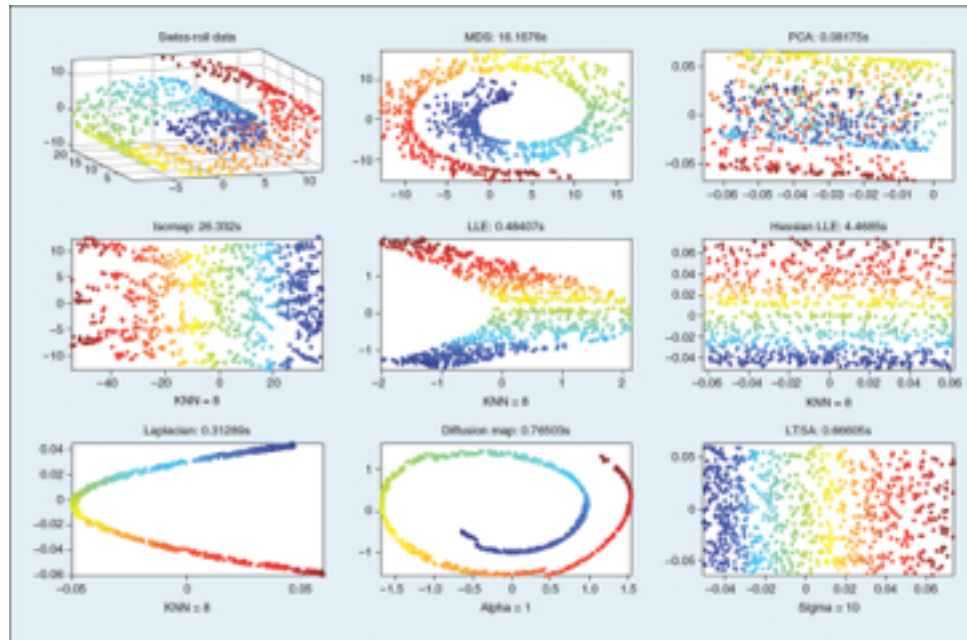
Zhang et al 2010

Many methods:
- Kernel PCA
- ISOMAP
- Local linear embedding
- Maximum volume unfolding
- Non-metric multidimensional scaling
- Laplacian
- Neural network auto encoder
- …

Due to lack of agreed upon metrics, it is very hard to judge which is best. Also, results from 3 to 2 dims is probably not representative of 1000 to 2 dimensions.

Other matrix factorizations

$$\mathbf{X} = \mathbf{U} \; \mathbf{S} \; \mathbf{V^T}$$

Singular value decomposition

$$\mathbf{U}^T\mathbf{U} = I, \; \mathbf{V}^T\mathbf{V} = I, \; \mathbf{S} = \operatorname{drag}(s)$$

$$\mathbf{U} \in \mathbb{R}^{n \times q}, \; \mathbf{V} \in \mathbb{R}^{m \times q}, \; s \in \mathbb{R}^{q}_{+}$$

$$\mathbf{X} \approx \mathbf{U}_q\mathbf{S}_q\mathbf{V}_q^T$$

Nonnegative matrix factorization (NMF)

$$\mathbf{W} \in \mathbb{R}^{n \times q}_{+} \text{ with } \mathbf{W1} = \mathbf{1}$$

$$\mathbf{B} \in \mathbb{R}^{q \times n}_{+} \text{ with } \mathbf{B1} = \mathbf{1}$$

$$\mathbf{X} \approx \mathbf{WBX}$$

PCA

Original

NMF
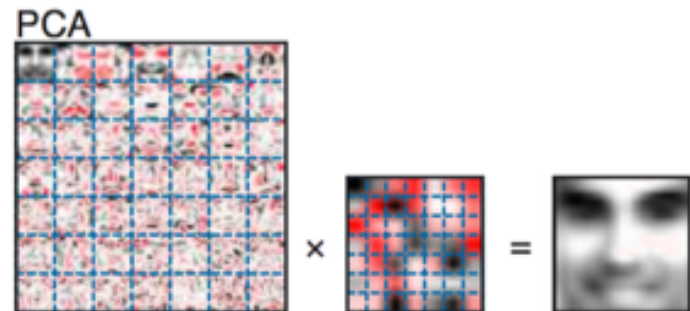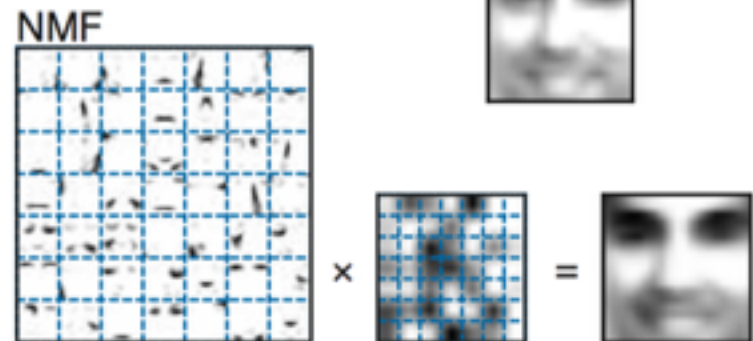
Clustering

Machine Learning – CSE546

Kevin Jamieson

University of Washington

November 16, 2016

Clustering images

C_1

C_2

C_3

C_4

C_5

[Goldberger et al.]

Set of Images
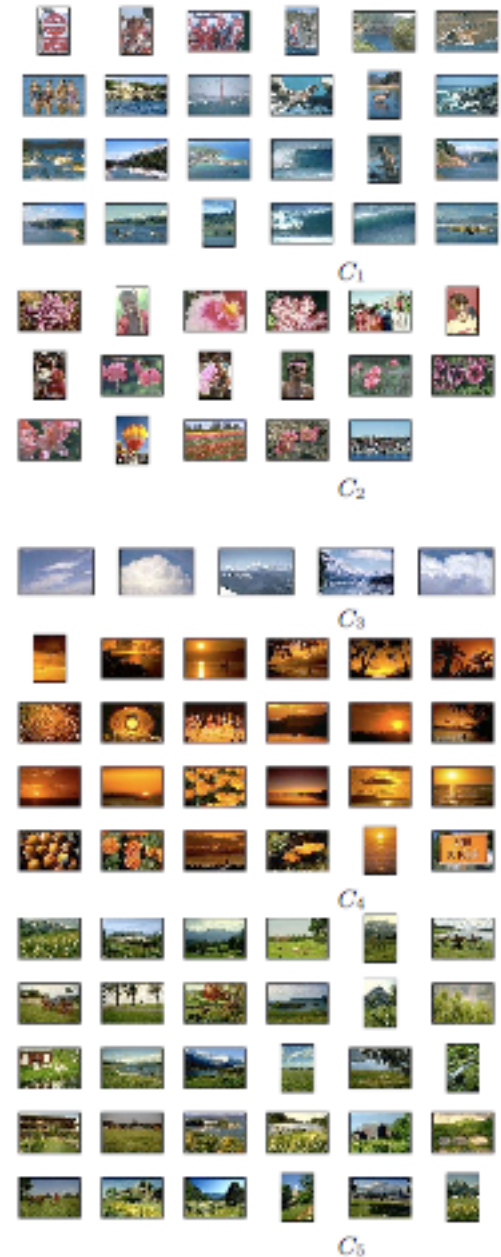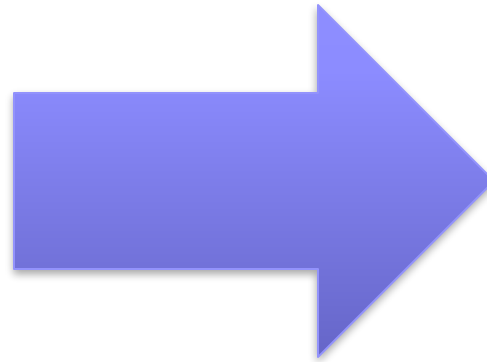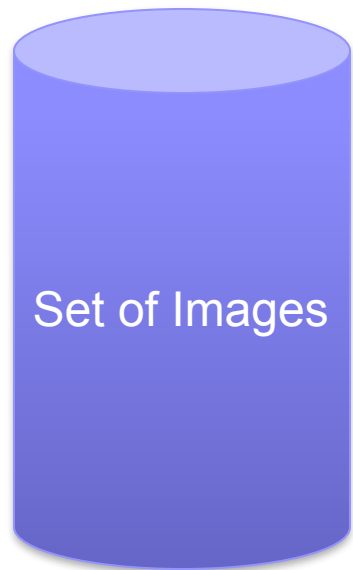
Clustering web search results

Hierarchical Clustering

Pick one:
- Bottom up: start with every point as a cluster and merge
- Top down: start with a single cluster containing all points and split

Different rules for splitting/merging, no "right answer"

Gives apparently interpretable tree representation. However, warning: even random data with no structure will produce a tree that "appears" to be structured.

Some Data

Auton's Graphics
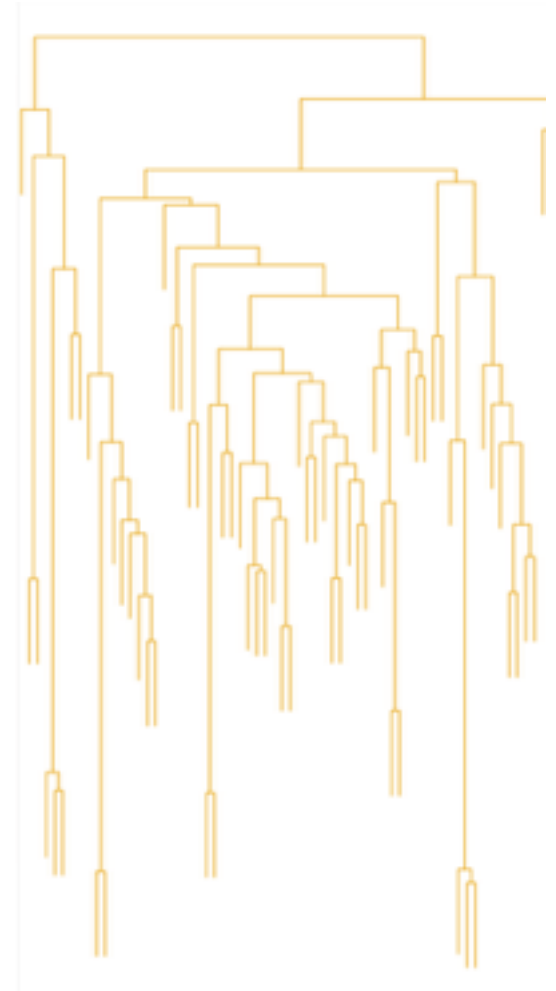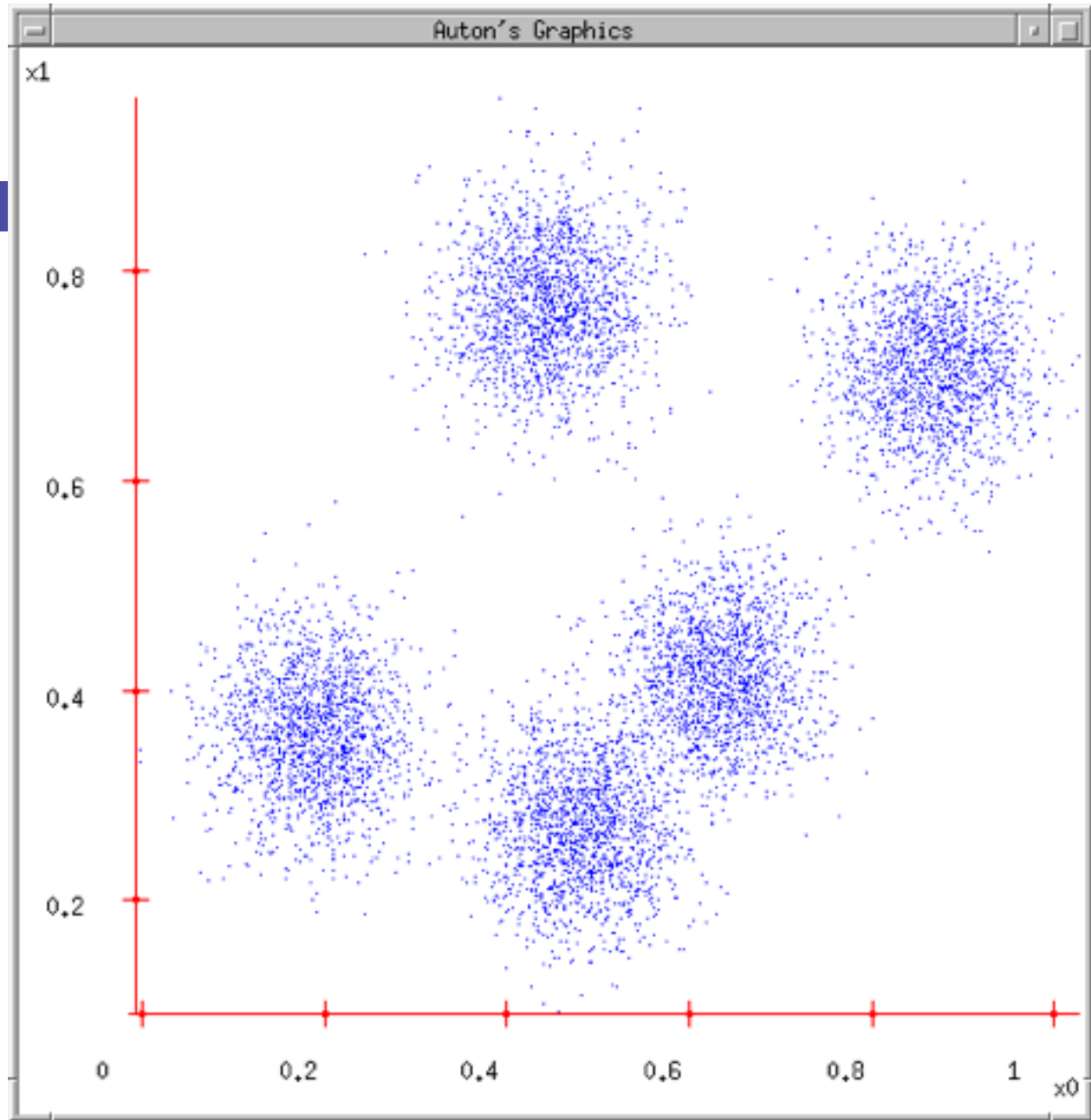
K-means

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

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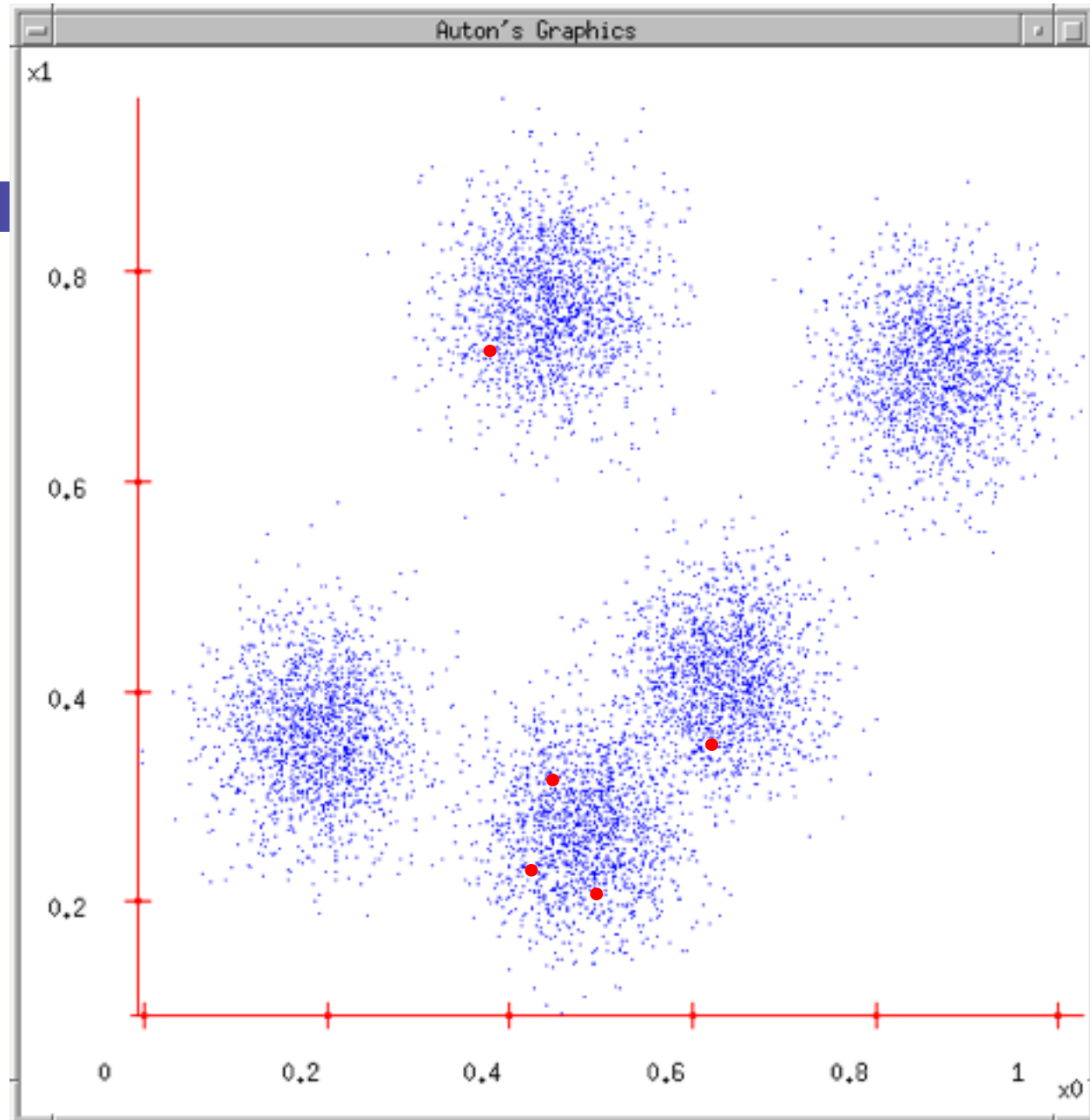
K-means

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

2. Randomly guess k cluster Center locations

3. Each datapoint finds out which Center it's closest to. (Thus each Center "owns" a set of datapoints)
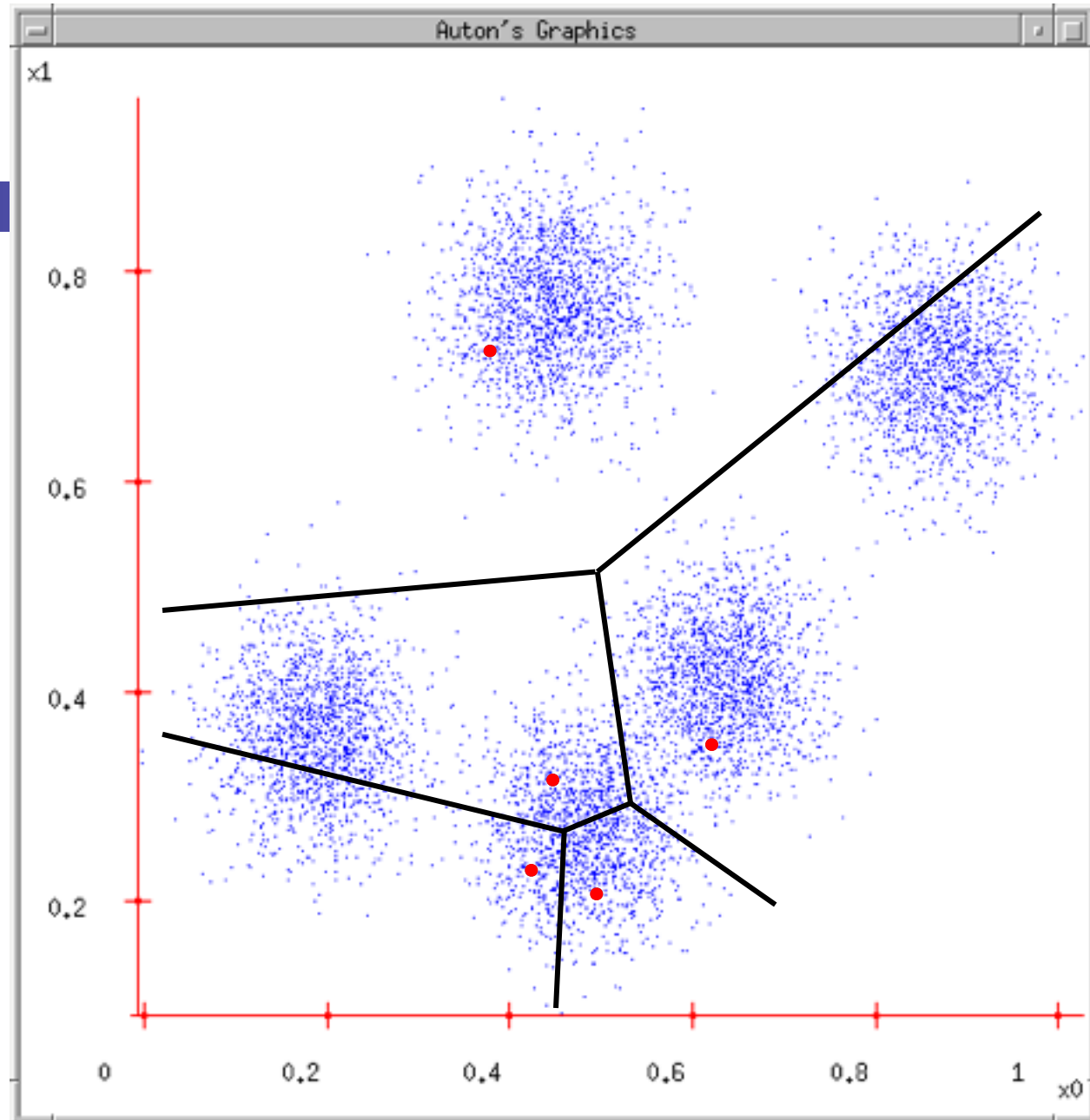
K-means

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3. Each datapoint finds out which Center it's closest to.

4. Each Center finds the centroid of the points it owns
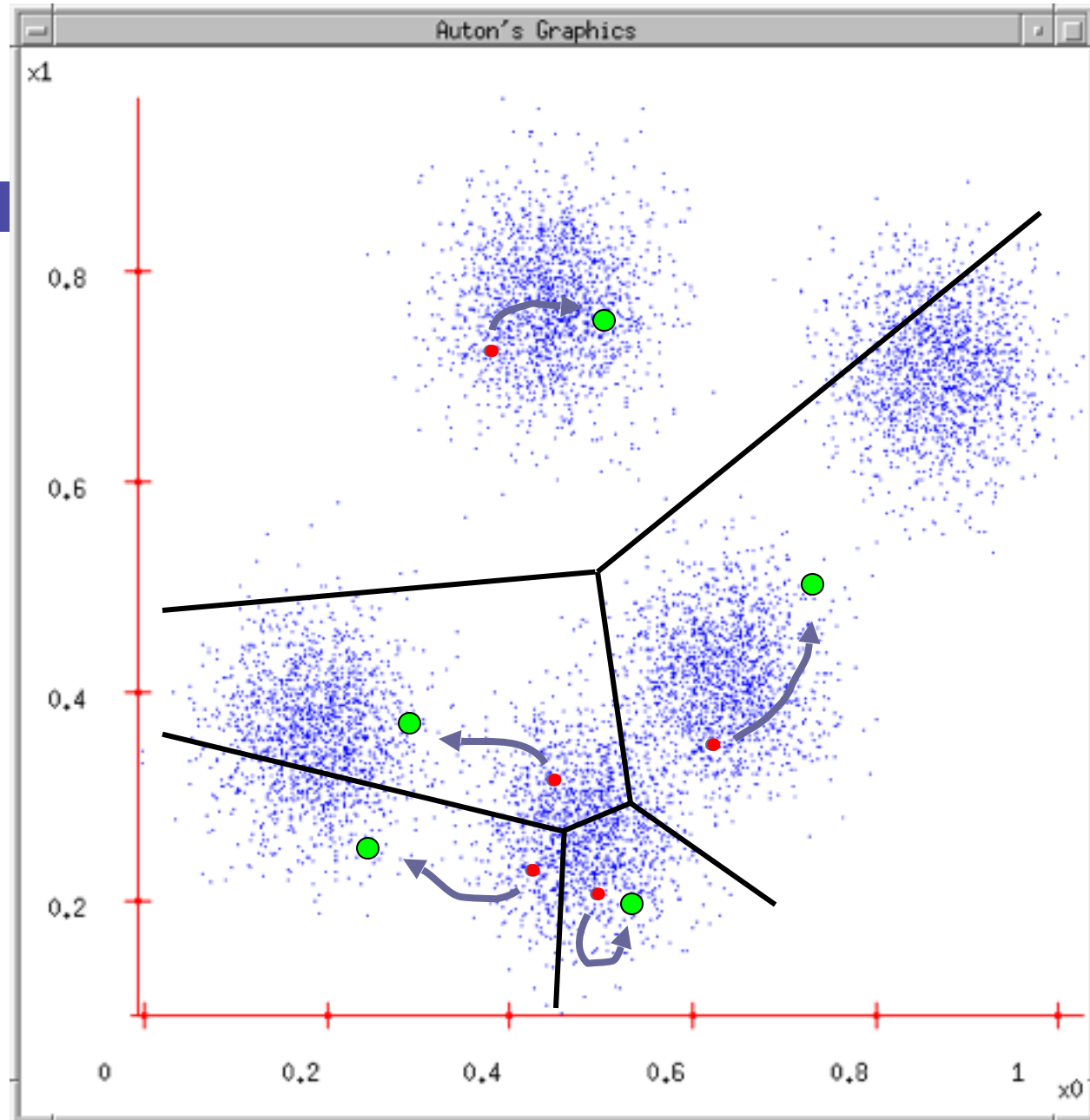
K-means

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

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4. Each Center finds the centroid of the points it owns…

5. …and jumps there

6. …Repeat until terminated!

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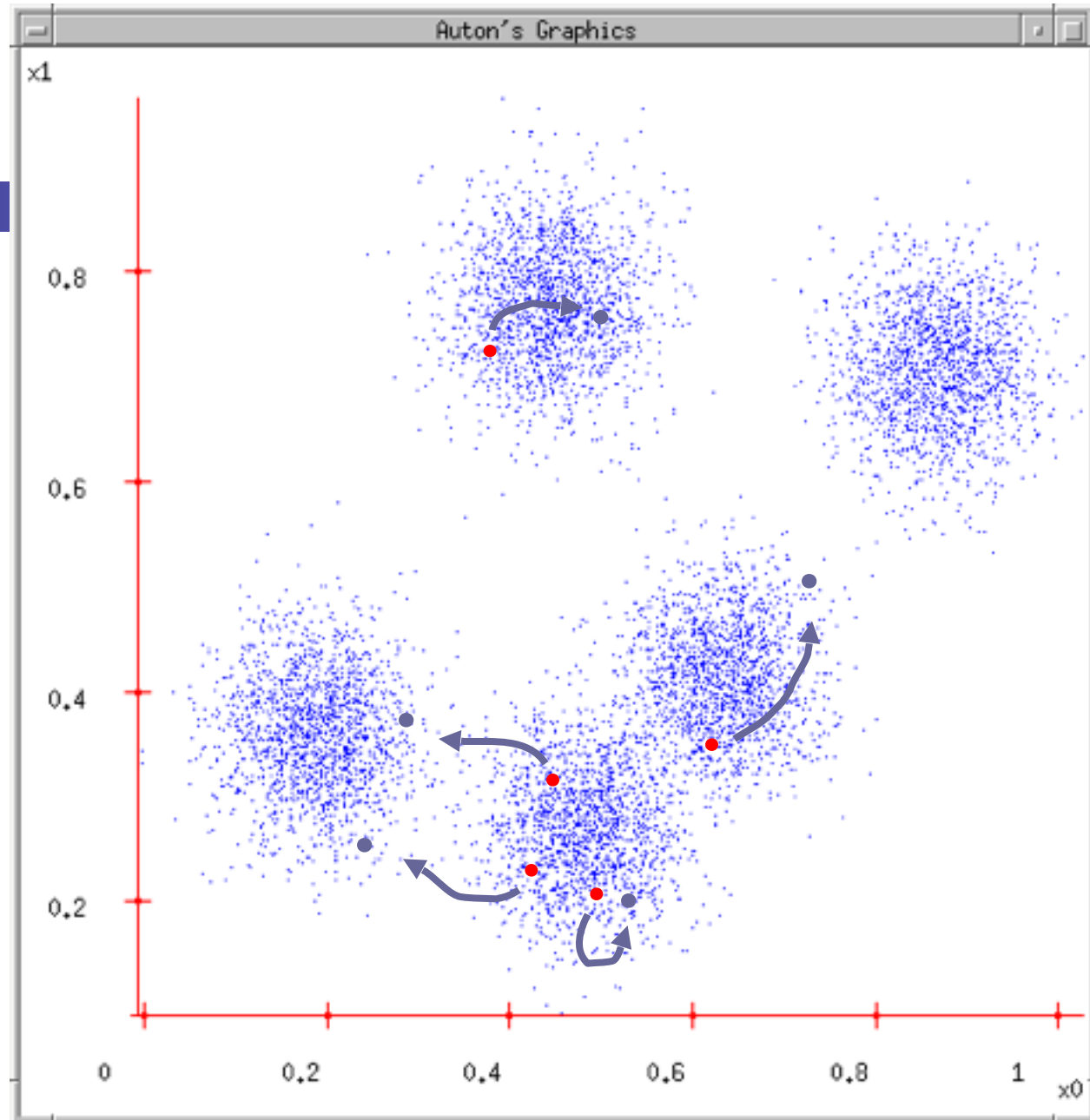
K-means

- Randomly initialize k centers
  - $\mu^{(0)} = \mu_1^{(0)}, \ldots, \mu_k^{(0)}$

- **Classify**: Assign each point $j \in \{1, \ldots N\}$ to nearest center:
  - $$C^{(t)}(j) \leftarrow \arg\min_i \|\mu_i - x_j\|^2$$

- **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 its points!

What is K-means optimizing?

- Potential function F(μ,C) of centers μ and point allocations C:

  $$F(\mu, C) = \sum_{j=1}^{N} \|\mu_{C(j)} - x_j\|^2$$

- Optimal K-means:
  - $\min_\mu \min_C F(\mu,C)$

Does K-means converge??? Part 1

- Optimize potential function:

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

- Fix μ, optimize C

Does K-means converge??? Part 2

- Optimize potential function:

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

- Fix C, optimize μ

Vector Quantization, Fisher Vectors

Vector Quantization (for compression)

1. Represent image as grid of patches
2. Run k-means on the patches to build code book
3. Represent each patch as a code word.

FIGURE 14.9. *Sir Ronald A. Fisher (1890 − 1962) was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a 1024×1024 grayscale image at 8 bits per pixel. The center image is the result of 2 × 2 block VQ, using 200 code vectors, with a compression rate of 1.9 bits/pixel. The right image uses only four code vectors, with a compression rate of 0.50 bits/pixel*

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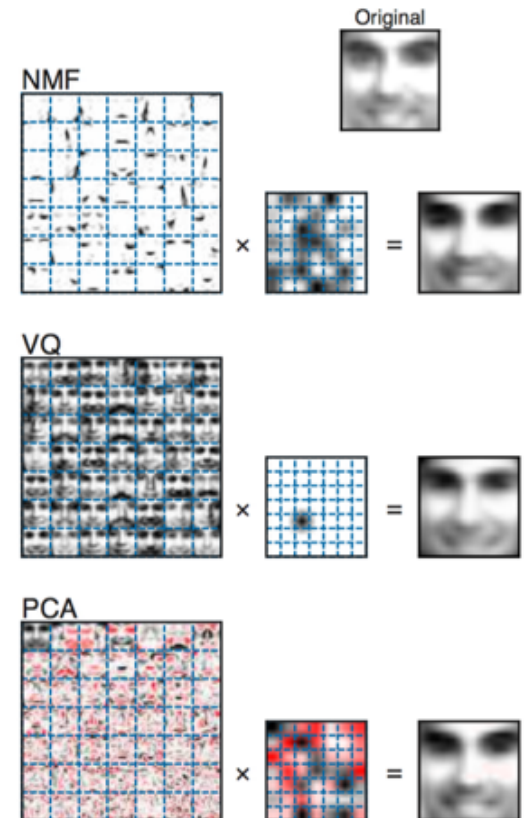
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Typical output of k-means
on patches
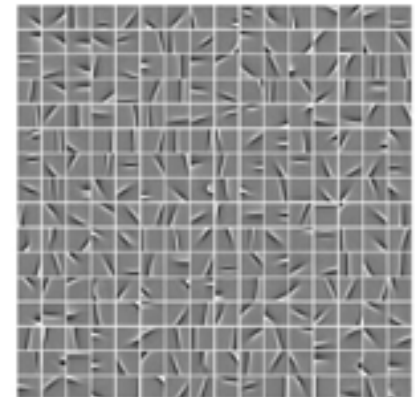
Similar reduced representation can be used as a feature vector

Coates, Ng, *Learning Feature Representations with K-means,* 2012
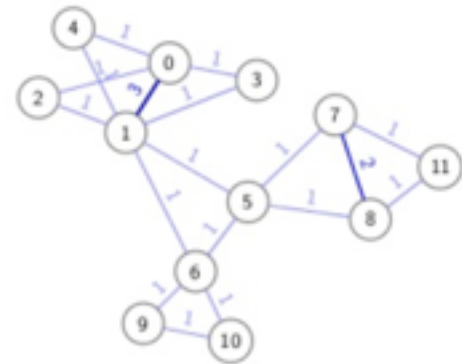
Spectral Clustering

Adjacency matrix: $\mathbf{W}$

$\mathbf{W}_{i,j} = $ weight of edge (i,j)

$$\mathbf{D}_{i,i} = \sum_{j=1}^{n} \mathbf{W}_{i,j} \qquad \mathbf{L} = \mathbf{D} - \mathbf{W}$$

Given feature vectors, could construct:
- k-nearest neighbor graph with weights in {0,1}
- weighted graph with arbitrary *similarities* $\mathbf{W}_{i,j} = e^{-\gamma||x_i - x_j||^2}$

Let $f \in \mathbb{R}^n$ be a function over the nodes

$$
\begin{aligned}
\mathbf{f}^T \mathbf{L} \mathbf{f} &= \sum_{i=1}^{N} g_i f_i^2 - \sum_{i=1}^{N} \sum_{i'=1}^{N} f_i f_{i'} w_{ii'} \\
&= \frac{1}{2} \sum_{i=1}^{N} \sum_{i'=1}^{N} w_{ii'} (f_i - f_{i'})^2.
\end{aligned}
$$

Spectral Clustering

Adjacency matrix: $\mathbf{W}$

$\mathbf{W}_{i,j} = $ weight of edge (i,j)

$\mathbf{D}_{i,i} = \sum\limits_{j=1}^{n} \mathbf{W}_{i,j}$ $\qquad \mathbf{L} = \mathbf{D} - \mathbf{W}$

Given feature vectors, could construct:
- (k=10)-nearest neighbor graph with weights in {0,1}

Popular to use the Laplacian $\mathbf{L}$ or its normalized form $\widetilde{\mathbf{L}} = I - \mathbf{D}^{-1}\mathbf{W}$ as a regularizer for learning over graphs