Clustering
K-means

UNIVERSITY *of* WASHINGTON

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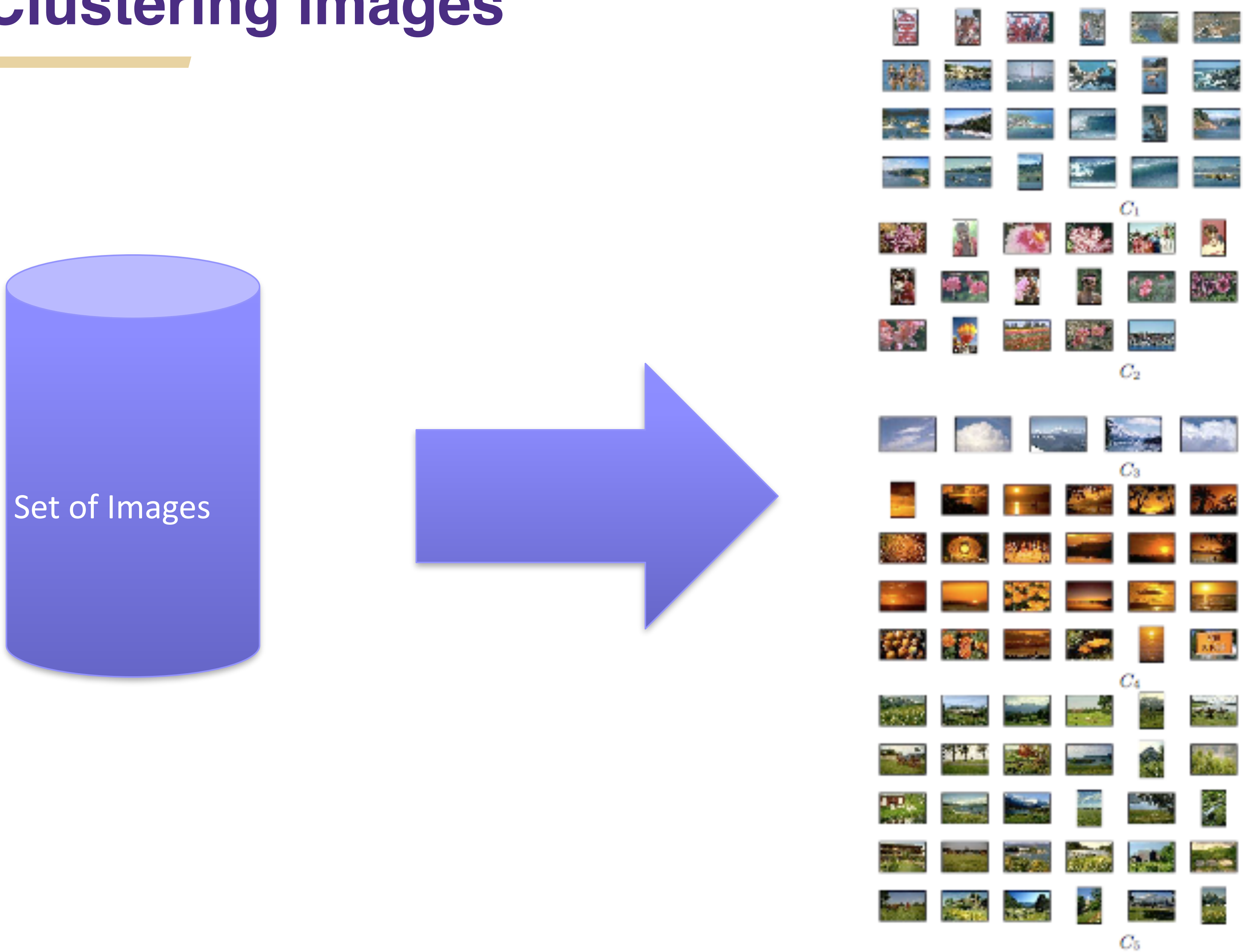
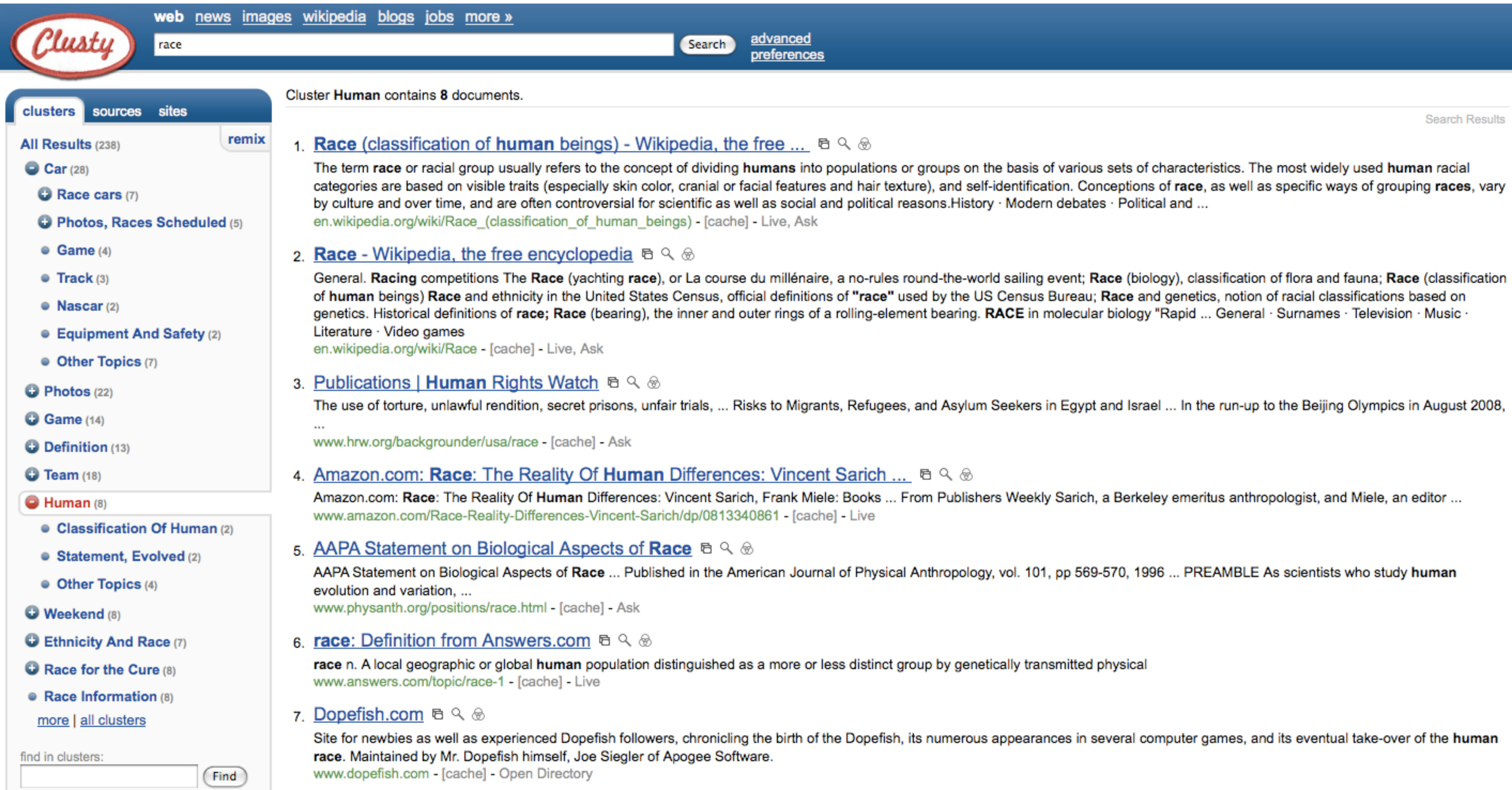
Clustering images

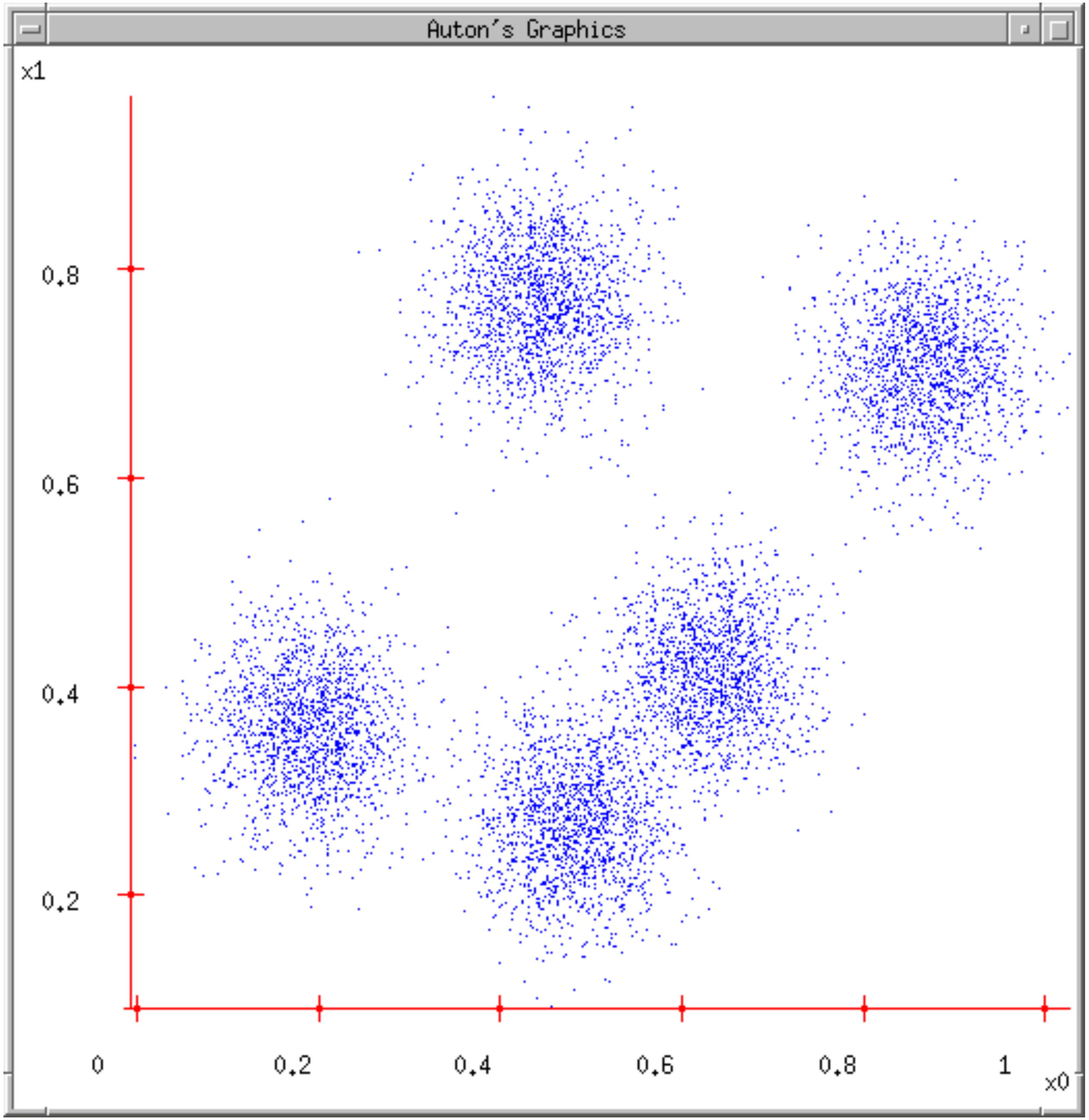


[Goldberger et al.]

Clustering web search results

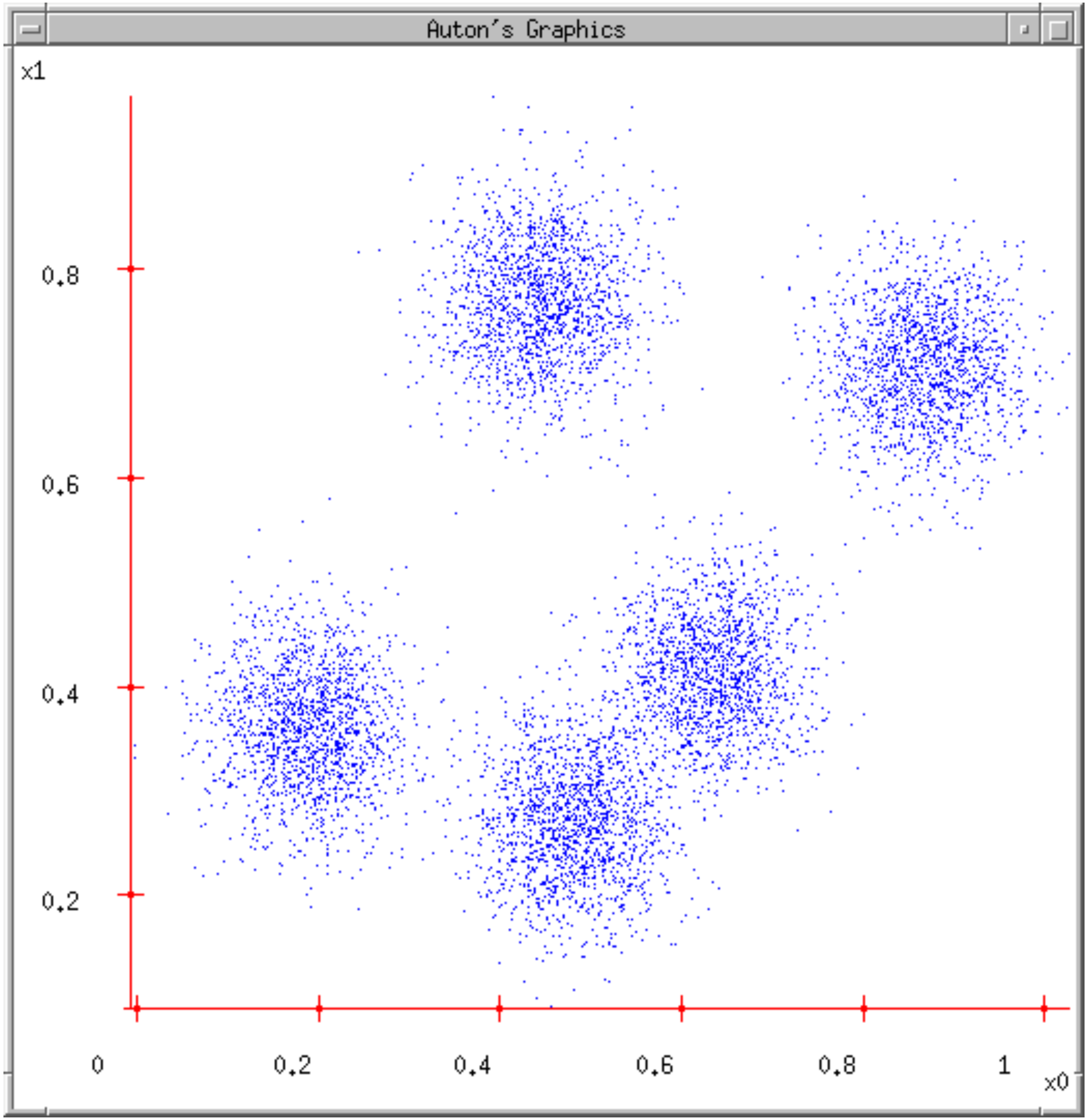


Some Data



Clustering

1. Ask user how many clusters they'd like. *(e.g. k=5)*
2. Pick clusters to minimize some objective fn.



Clustering

1. Fix a # of clusters *(e.g. k=5)*
2. Choose/Assign each point x_j to $C(j) \in \{1, \ldots, k\}$
   1. Sometimes, pick centers $\boldsymbol{\mu}_1 , \ldots \boldsymbol{\mu}_k$

   To minimize

$$F(\mu, C)$$

K-means refers to optimizing this objective:

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

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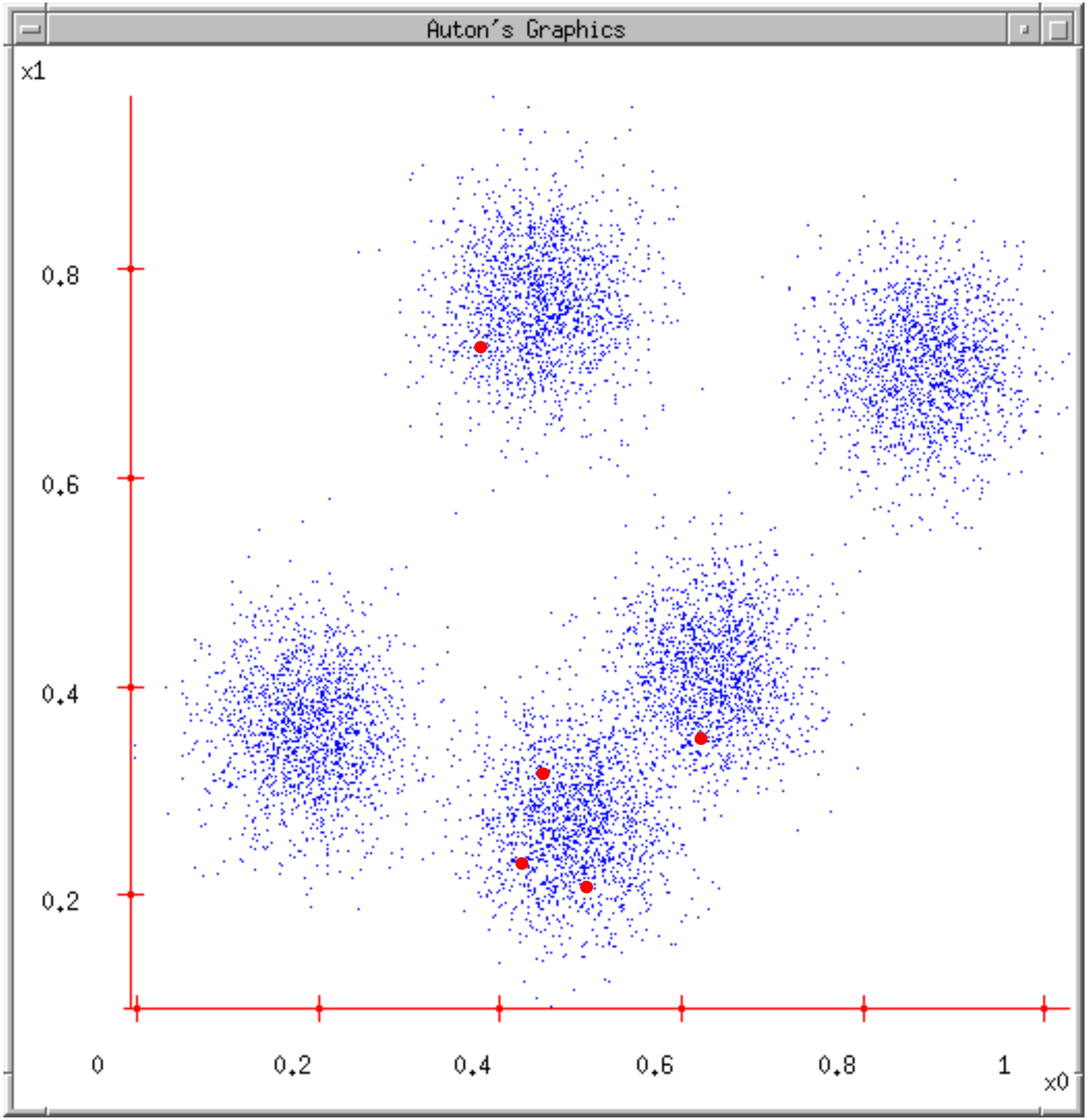
But, several natural algorithms work well in practice!

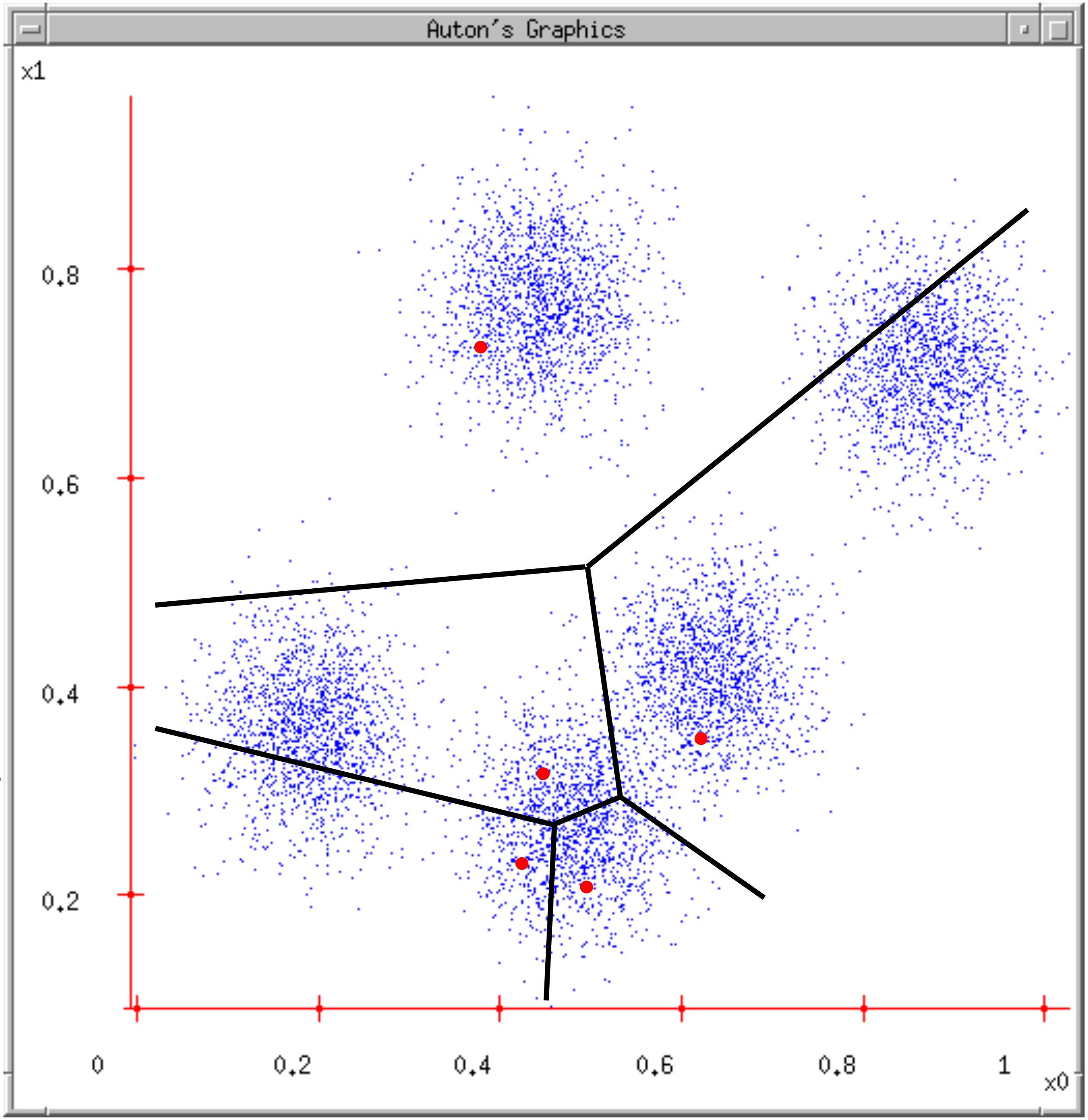
Lloyd's algorithm

1. Ask user how many clusters they'd like. *(e.g. k=5)*
2. Randomly guess k cluster Center locations



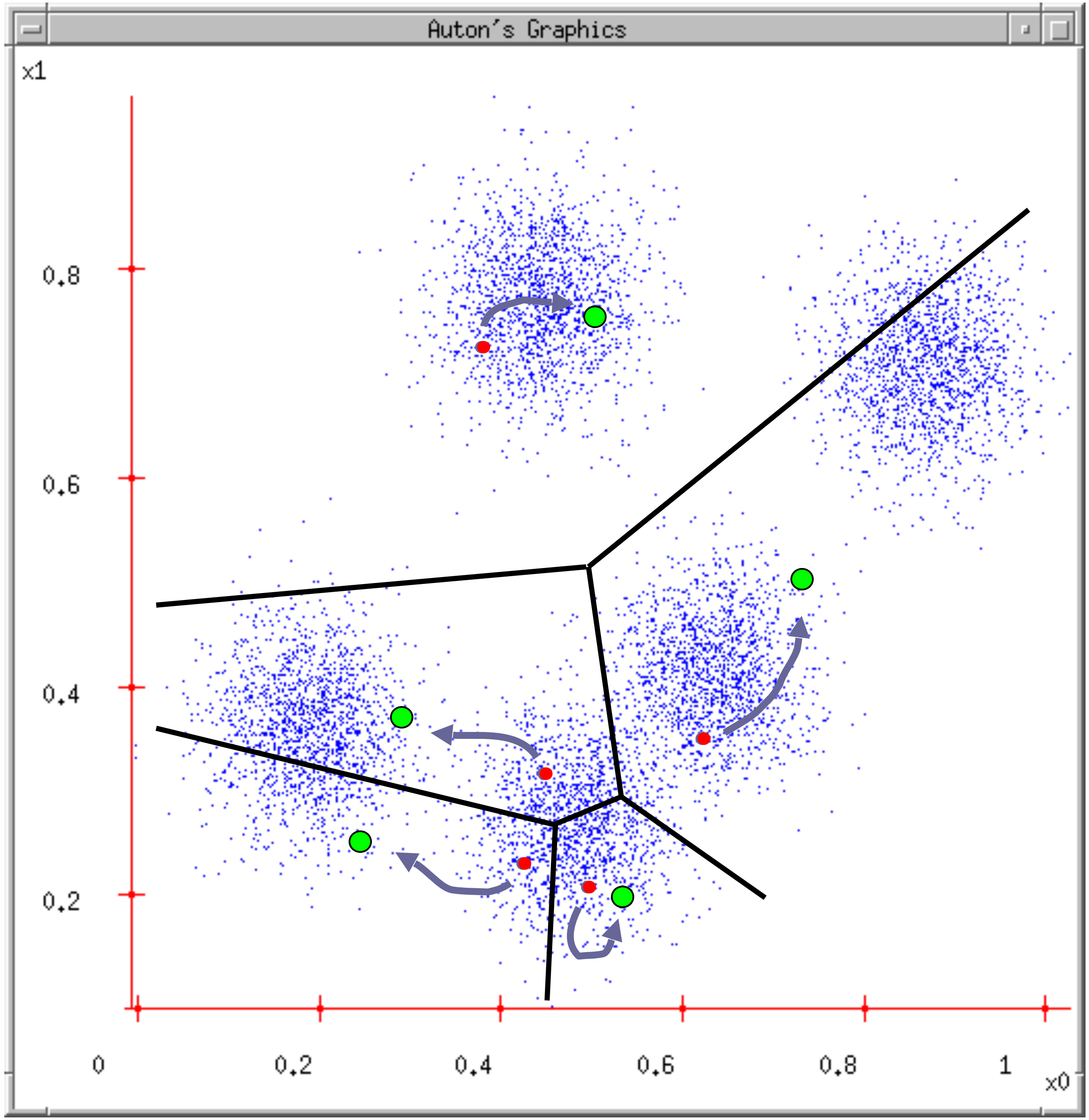
Lloyd's algorithm

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. (Each center "owns" a set of datapoints)



Lloyd’s algorithm

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



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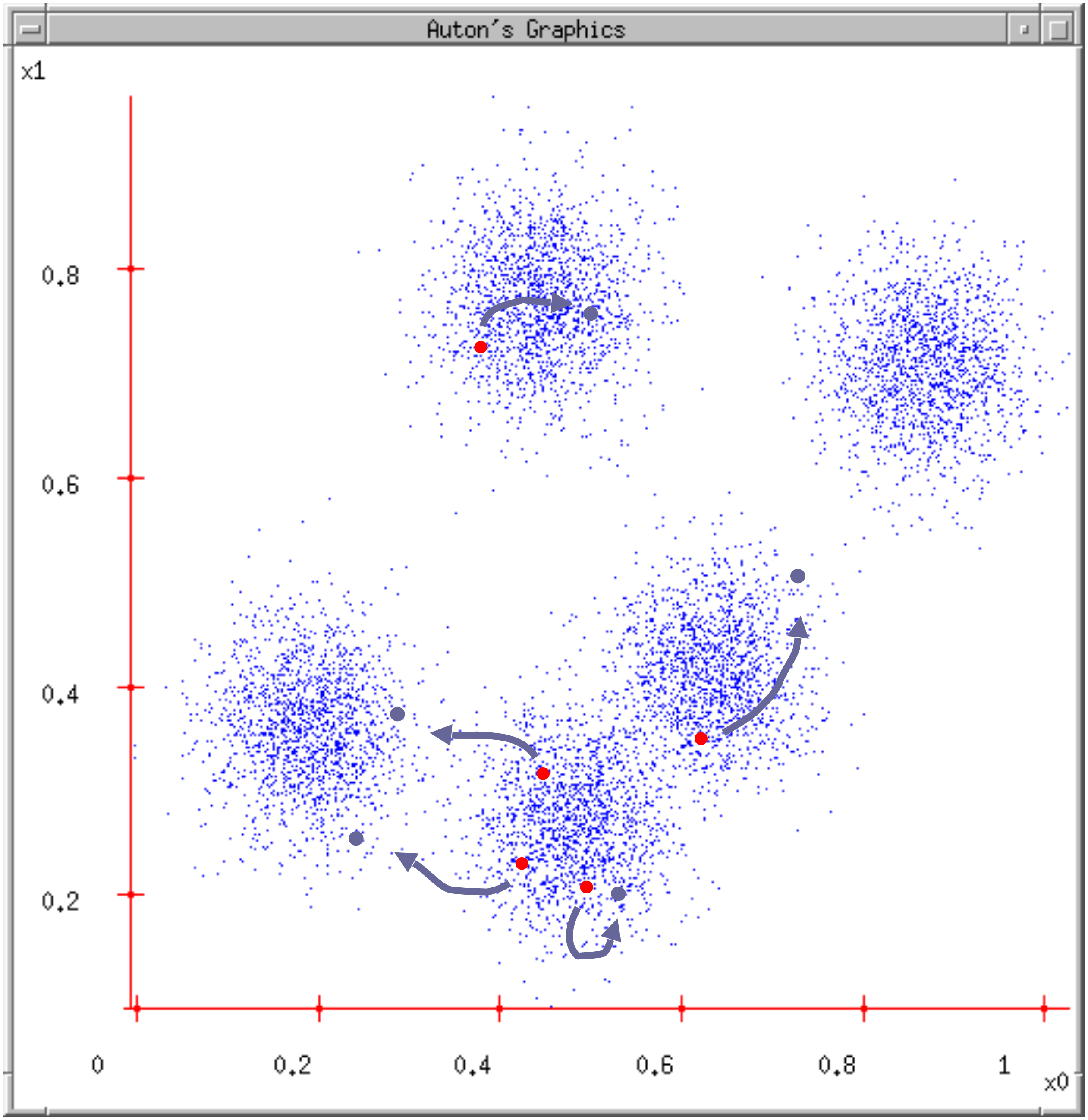
4. Each Center finds the centroid of the points it owns…
5. …and jumps there
6. …Repeat until terminated!



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$$C^{(t)}(j) \leftarrow \arg\min_i ||\mu_i - x_j||^2$$

$$\mu_i^{(t+1)} \leftarrow \arg\min_{\mu} \sum_{j:C(j)=i} ||\mu - x_j||^2$$

Does Lloyd's algorithm converge??? Part 1

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

First, fix **μ**

minimize w.r.t C

Does Lloyd’s algorithm converge??? Part 2

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

First, fix **μ**

minimize w.r.t C

Then, fix C

minimize w.r.t **μ**

$F(\mu, C)$ decreases each step $\Rightarrow$ the algorithm doesn’t cycle

Only $\binom{n}{k} \approx n^k$ configuarations $\Rightarrow$ converges in finite # iterations

A cool application of k-means clustering: compression

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*

Vector Quantization, Fisher Vectors

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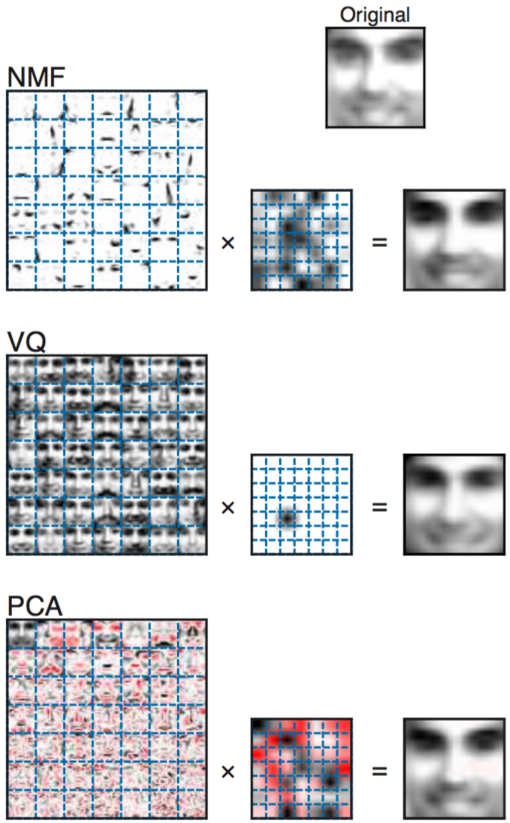

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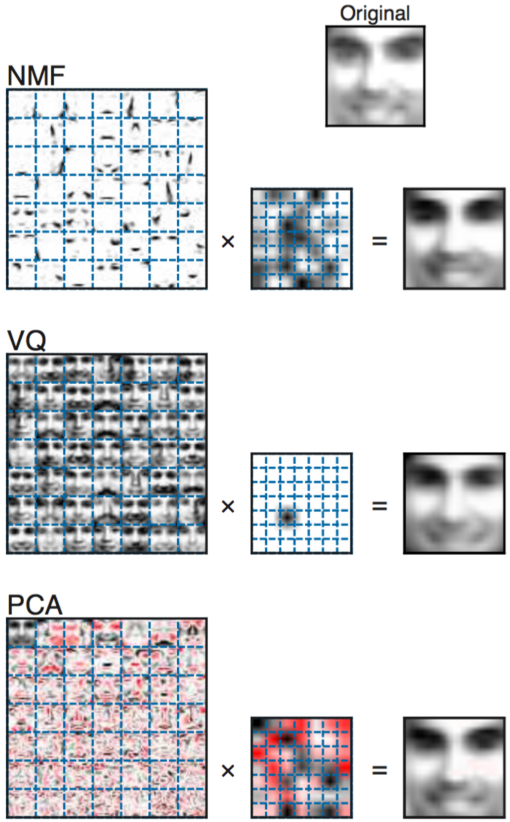

Coates, Ng, *Learning Feature Representations with K-means*, 2012

When to use K-means, or something else?

What sort of groupings are desired?

- Nonoverlapping, similar diameter clusters: k-means may work well
- Otherwise, might want another objective function (spectral, k-median, k-mode, …)

One bad case for k-means

K-means summary

A clustering objective

minimize average L2 distance to centers of clusters

Lloyd's algorithm: a greedy heuristic for minimizing it

Will converge in finite time, may not find global minimum

Good for finding similar width, nonoverlapping clusters

Sensitive to initial center selection, and random may not be the best a priori

See k-means++, *The Advantages of Careful Seeding,* Arthur and Vassilvitskii

Principal Component Analysis

Figure credit:

Karlin
Roughgarden + Valiant
Benedetto
Novembre et al
Alex Williams
Sandipan Dey
Victor Lavenko

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PCA

Data dependent dimensionality reduction

- Useful for
  - Visualization
  - Interpretation
  - Compression
  - Understanding “intrinsic dimension”

	kale	taco bell	sashimi	pop tarts
Alice	10	1	2	7
Bob	7	2	1	10
Carolyn	2	9	7	3
Dave	3	6	10	2

Figure credit:
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PCA

Claim:

Each row can be expressed approximately as

$$x_i \approx \bar{x} + a_{i1}\vec{v_1} + a_{i2}\vec{v_2}$$

$$\vec{v_1} = [3 \quad -3 \quad -3 \quad 3]$$

$$\vec{v_2} = [1 \quad -1 \quad 1 \quad -1]$$

	kale	taco bell	sashimi	pop tarts
Alice	10	1	2	7
Bob	7	2	1	10
Carolyn	2	9	7	3
Dave	3	6	10	2

$$\bar{x} = [5.5 \quad 4.5 \quad 5 \quad 5.5]$$

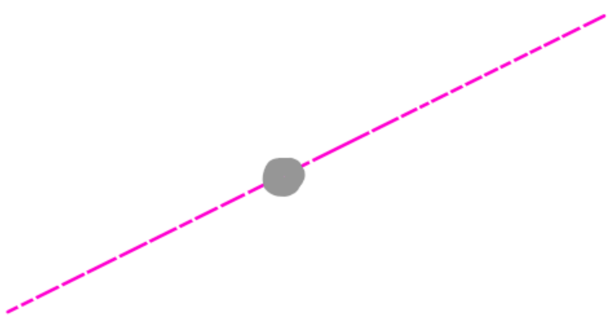
PCA in one dimension

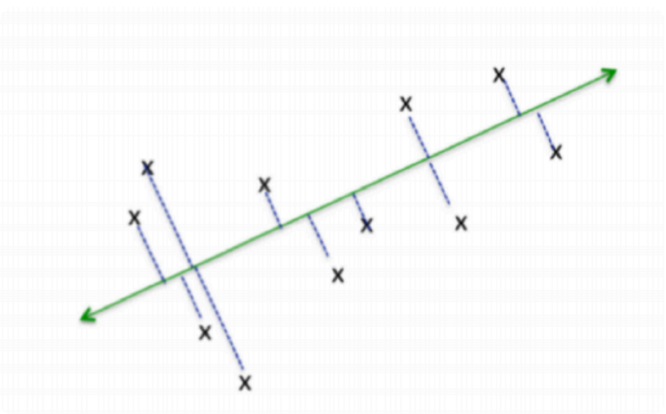
Goal: find a k < d-dimensional representation of X

For k = 1:

Choose $\vec{v} \in \mathbb{R}^d, ||v|| = 1$
to minimize

$$\frac{1}{n}\sum_{i=1}^{n} dist(x_i, \text{line defined by } \vec{v})$$





PCA in one dimension, 2 equivalent views

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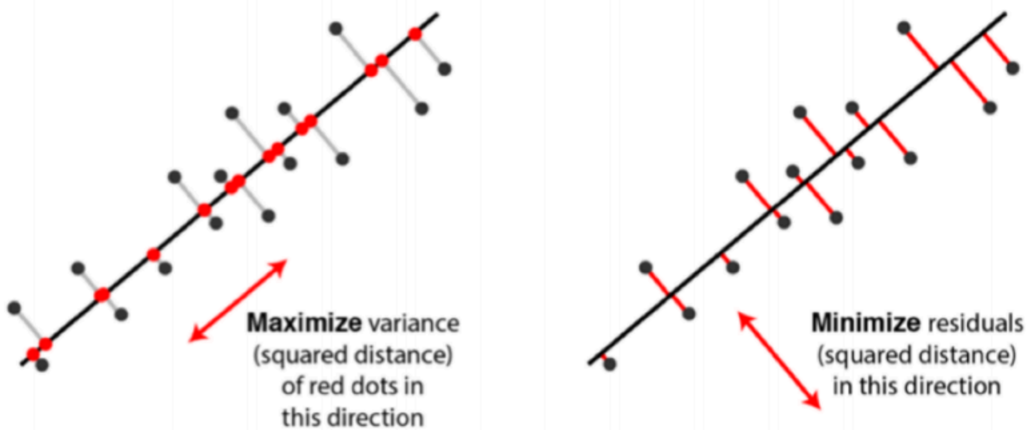

Two equivalent views of principal component analysis.

PCA: finding a linear projection

Given $x_1, \ldots, x_n \in \mathbb{R}^d$, for $q \ll d$ find a compressed representation with $\lambda_1, \ldots, \lambda_n \in \mathbb{R}^q$ such that $x_i \approx \mu + \mathbf{V}_q \lambda_i$ and $\mathbf{V}_q^T \mathbf{V}_q = I$

$$\min_{\mu, \mathbf{V}_q, \{\lambda_i\}_i} \sum_{i=1}^{n} \|x_i - \mu - \mathbf{V}_q \lambda_i\|_2^2$$

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$$\min_{\mu, \mathbf{V}_q, \{\lambda_i\}_i} \sum_{i=1}^{n} \|x_i - \mu - \mathbf{V}_q \lambda_i\|_2^2$$

Fix $\mathbf{V}_q$ and solve for μ, λ_i:

$$\mu = \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\lambda_i = \mathbf{V}_q^T (x_i - \bar{x})$$

Which gives us:

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

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

Linear projections

$$\sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2$$

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

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

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Eigenvalue decomposition

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

Minimize reconstruction error and capture the most variance in your data.

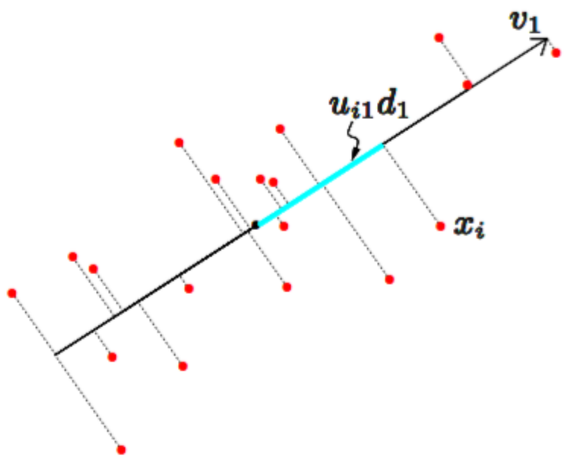
Linear projections

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 $\mathbf{V}_q$

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