ECE 5984: Introduction to Machine Learning

Topics:

- Unsupervised Learning: Kmeans, GMM, EM

Readings: Barber 20.1-20.3

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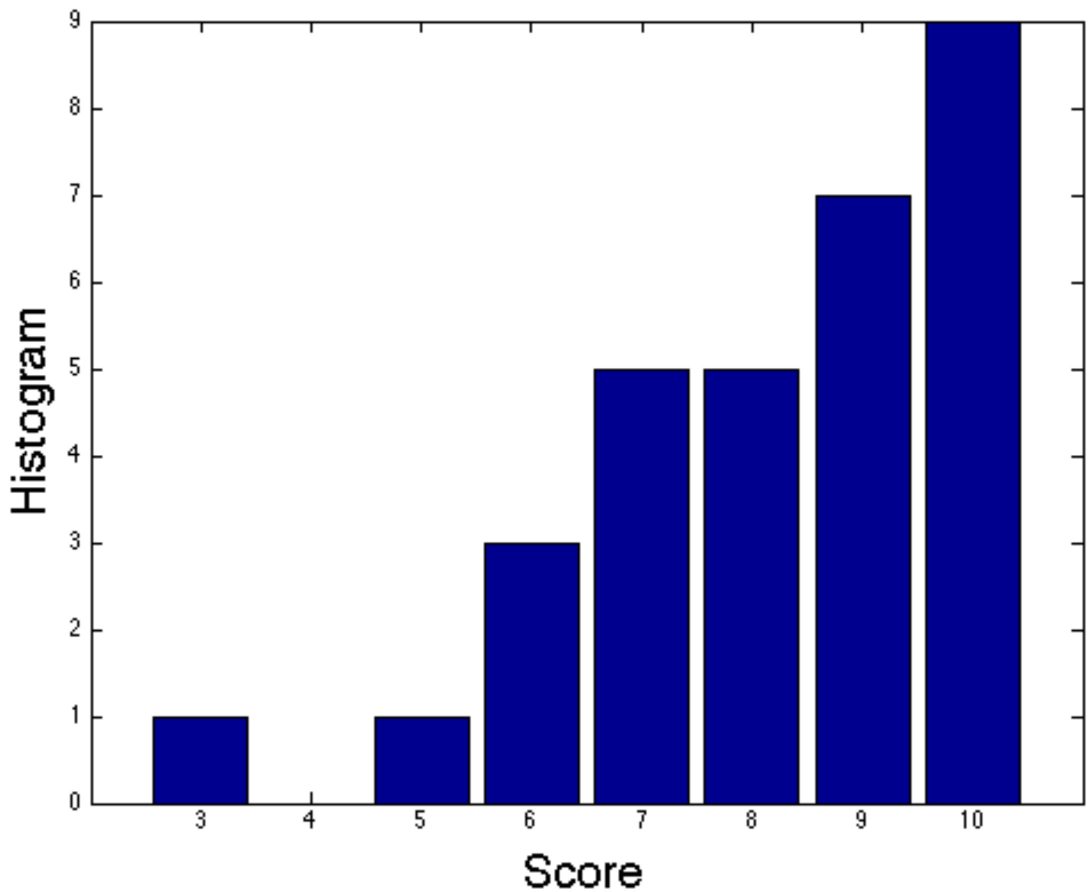
Virginia Tech

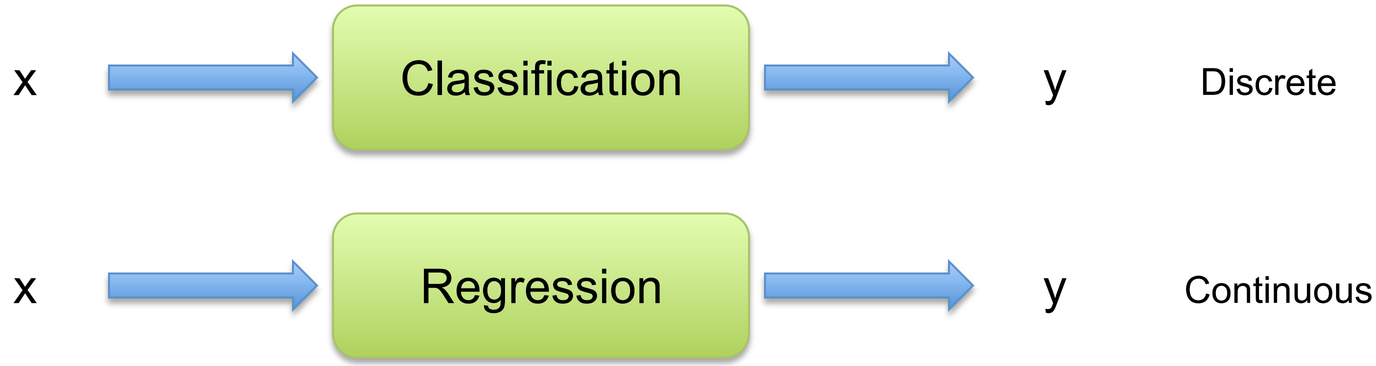
Midsem Presentations Graded

- Mean 8/10 = 80%
  - Min: 3
  - Max: 10

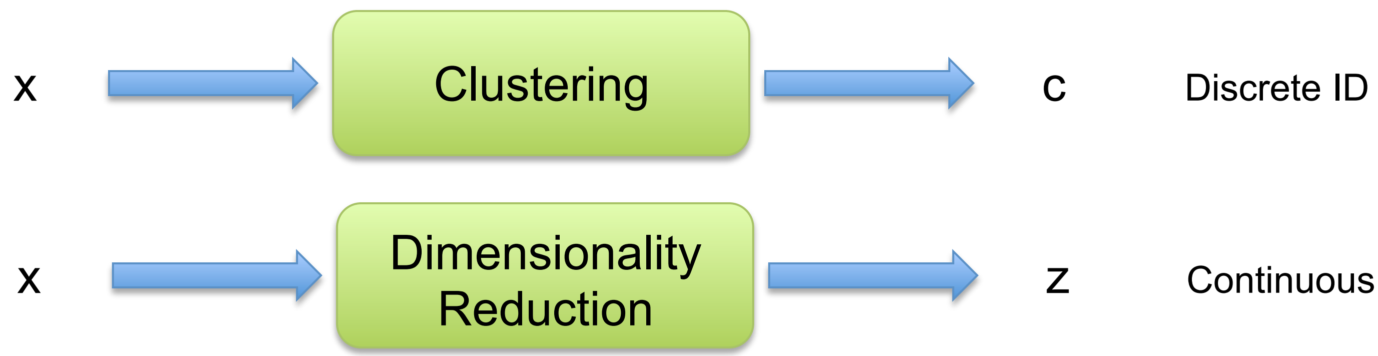


Tasks

Supervised Learning



Unsupervised Learning

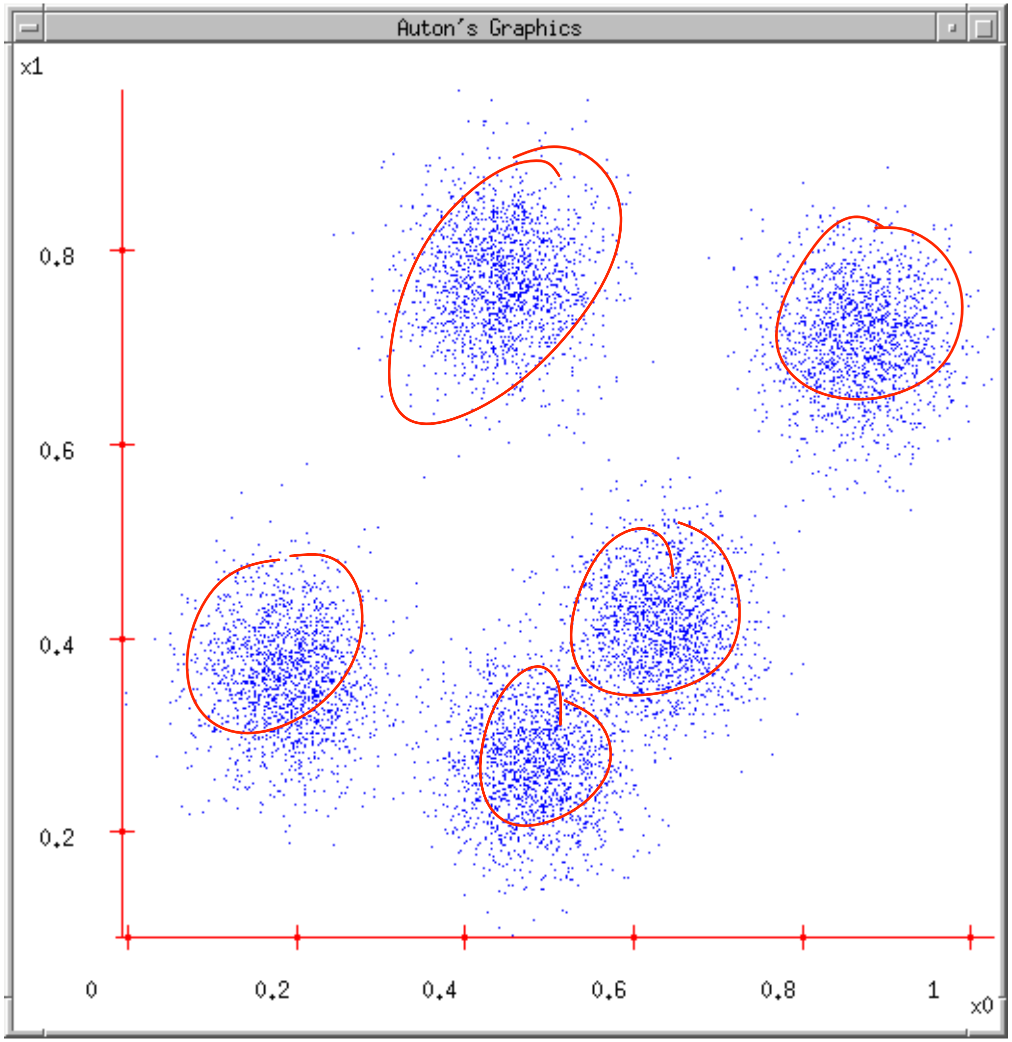


Unsupervised Learning

- Learning only with X
  - Y not present in training data

- Some example unsupervised learning problems:
  - Clustering / Factor Analysis
  - Dimensionality Reduction / Embeddings
  - Density Estimation with Mixture Models

New Topic: Clustering



Slide Credit: Carlos Guestrin

Synonyms

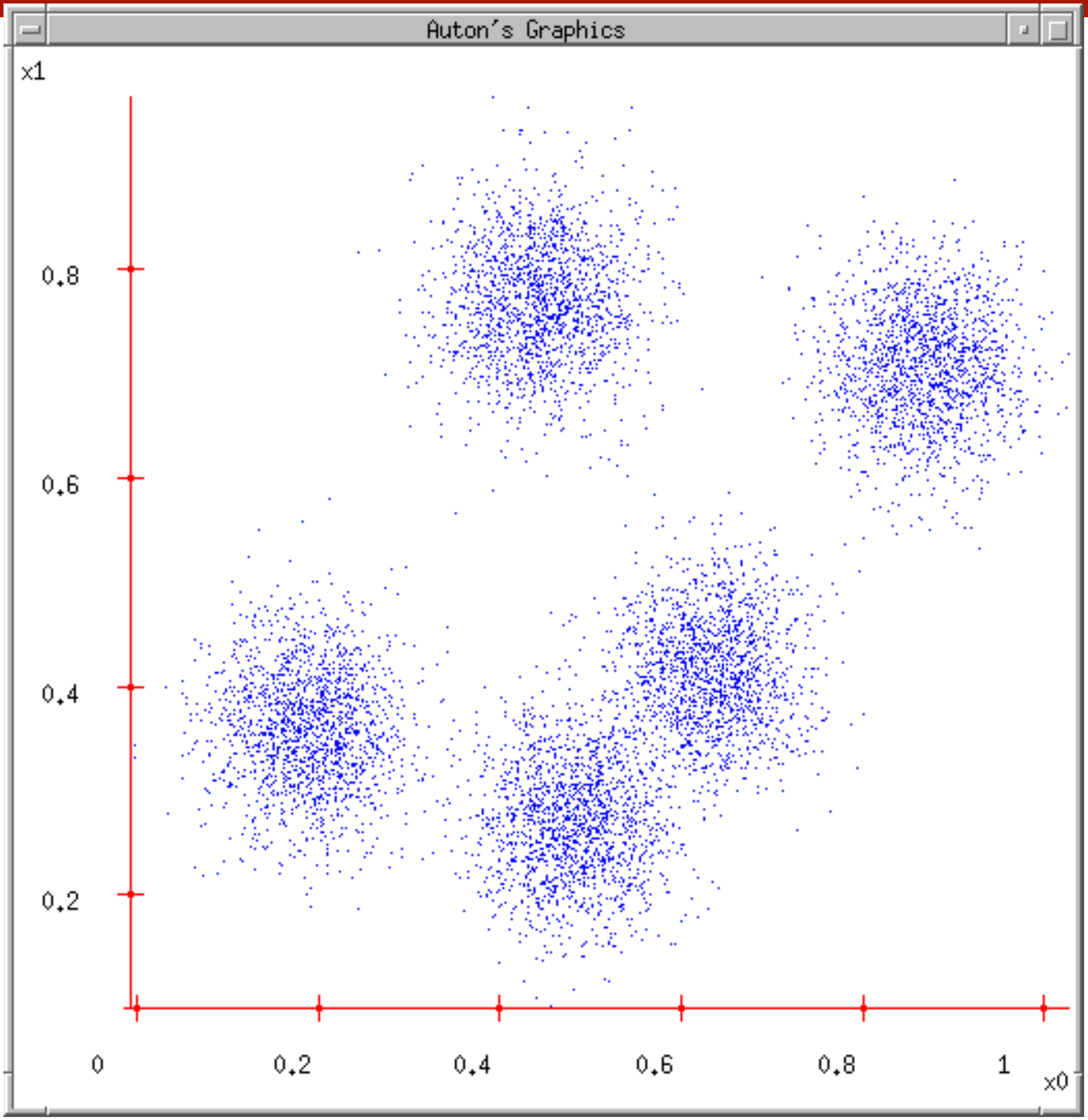
- Clustering

- Vector Quantization

- Latent Variable Models
- Hidden Variable Models
- Mixture Models

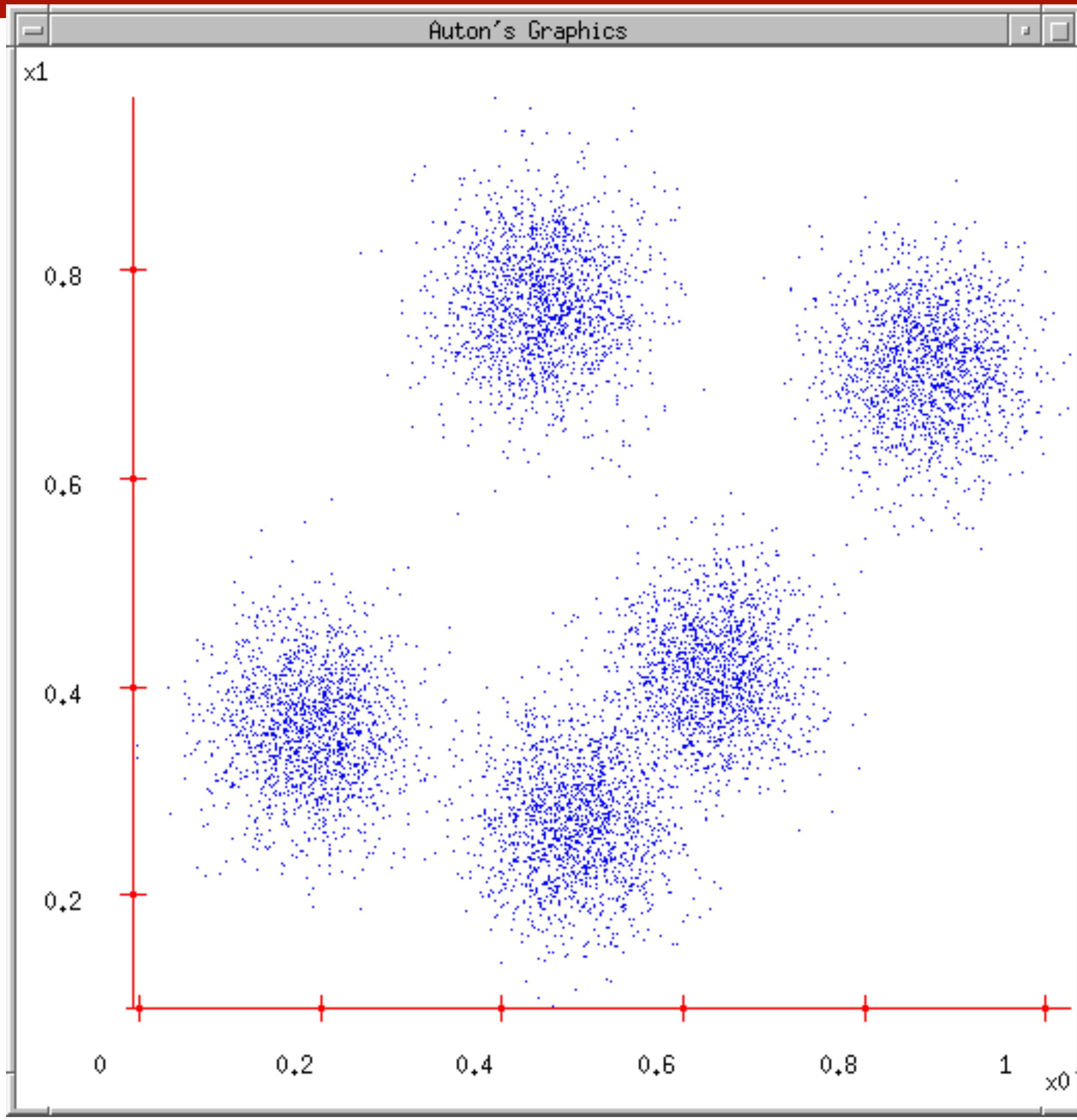
- Algorithms:
  - K-means
  - Expectation Maximization (EM)

Some Data



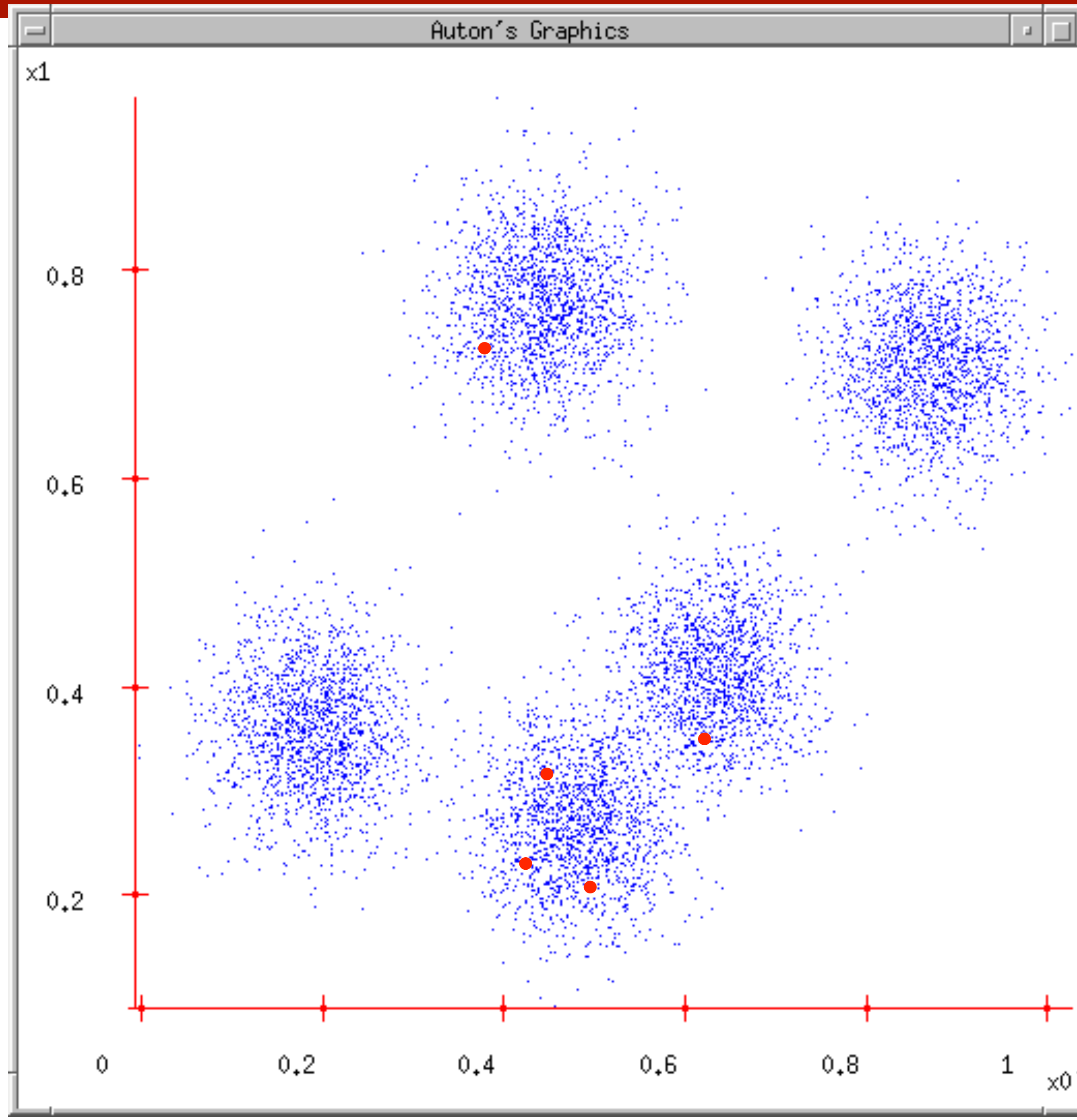
K-means

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



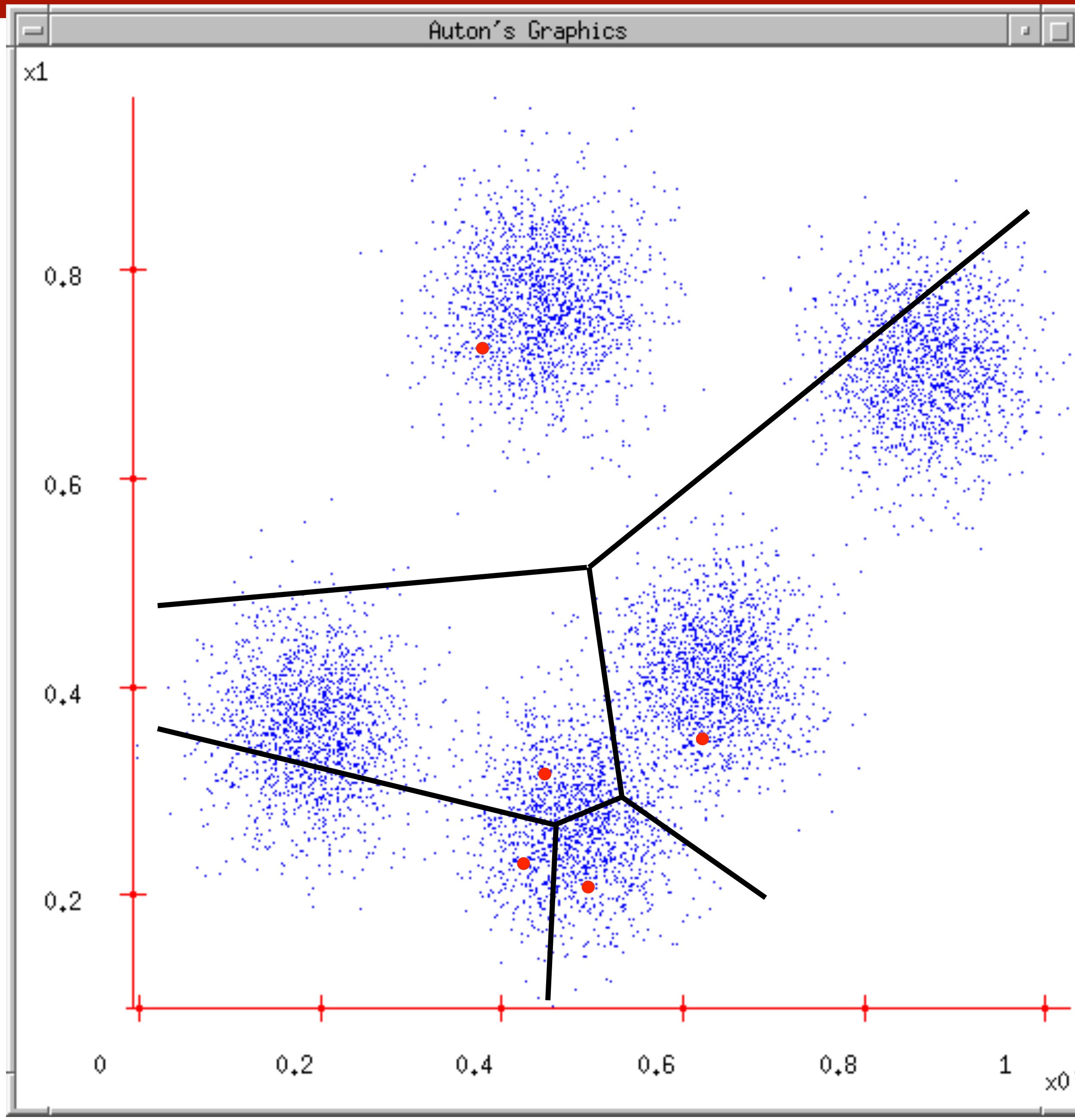
K-means

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



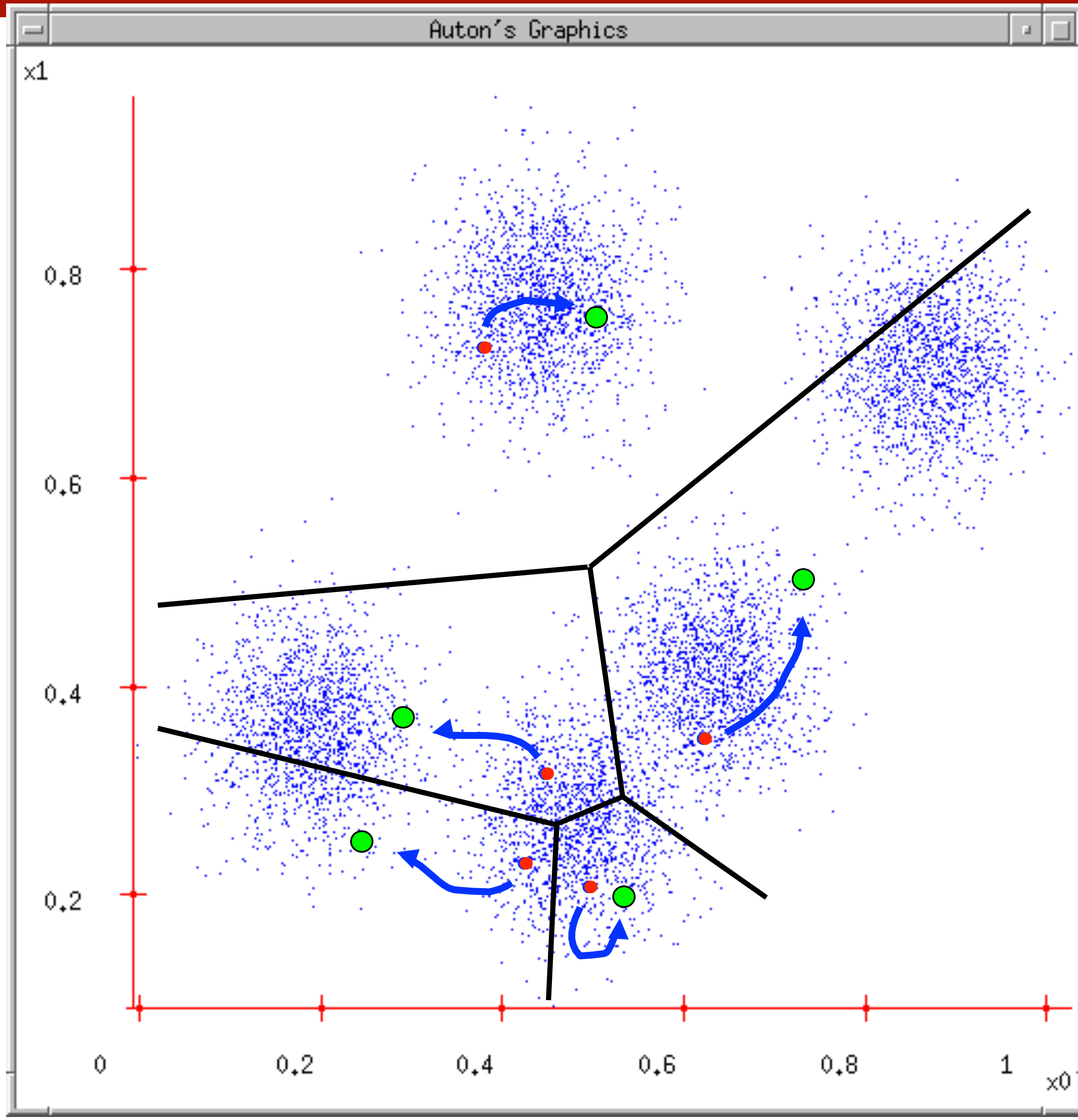
K-means

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)



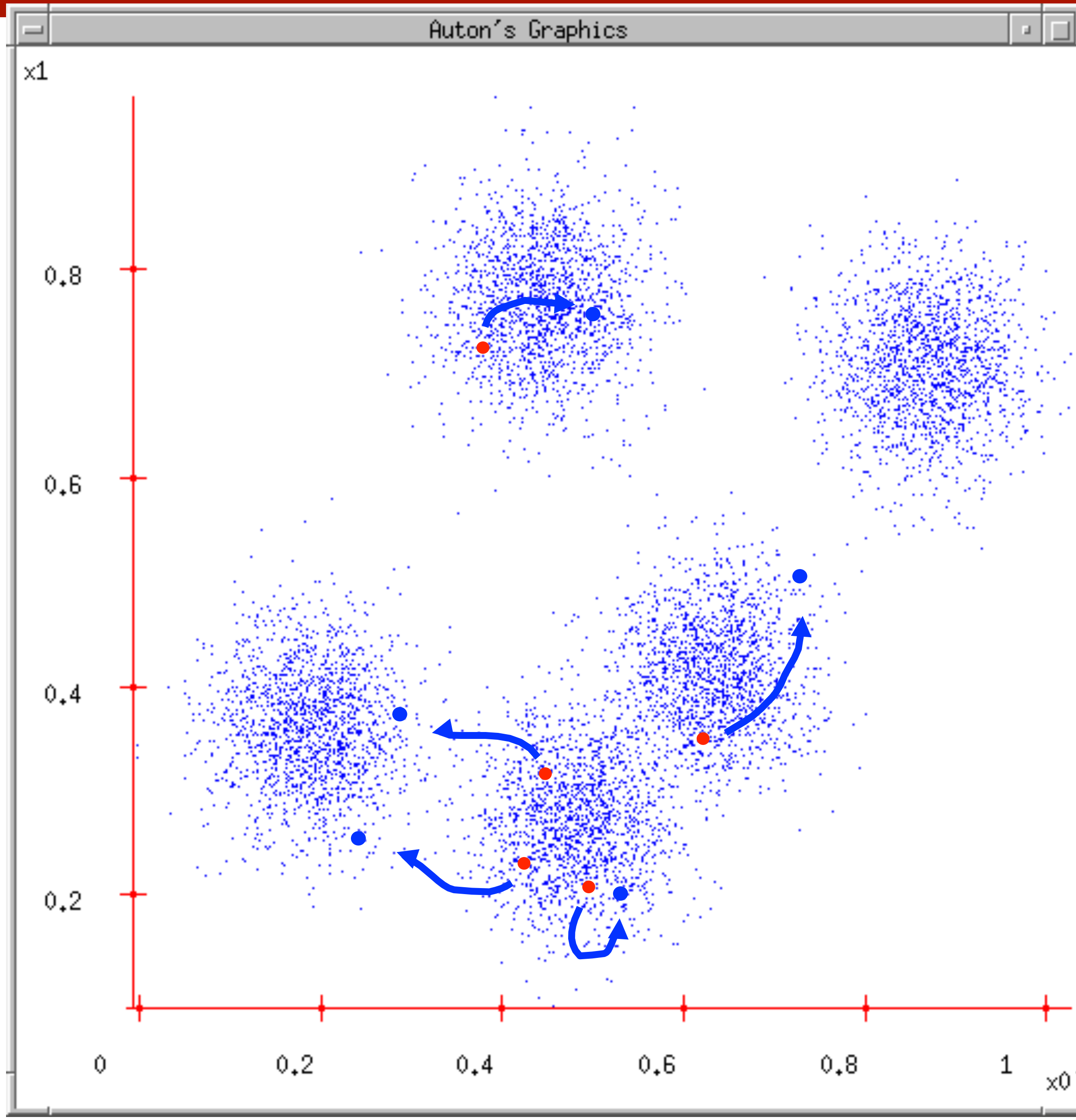
K-means

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



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.
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
  - $\mu^{(0)} = \mu_1^{(0)}, \ldots, \mu_k^{(0)}$

- **Assign**:
  - Assign each point $i \in \{1, \ldots n\}$ to nearest center:
  - $C(i) \longleftarrow \underset{j}{\operatorname{argmin}} ||\mathbf{x}_i - \boldsymbol{\mu}_j||^2$

- **Recenter**:
  - μ_j becomes centroid of its points

K-means

- Demo
  - http://www.kovan.ceng.metu.edu.tr/~maya/kmeans/
  - http://home.deib.polimi.it/matteucc/Clustering/tutorial_html/AppletKM.html

What is K-means optimizing?

- Objective F(μ,C): function of centers μ and point allocations C:
  - $F(\boldsymbol{\mu}, C) = \sum_{i=1}^{N} ||\mathbf{x}_i - \boldsymbol{\mu}_{C(i)}||^2$
  - 1-of-k encoding $F(\boldsymbol{\mu}, \boldsymbol{a}) = \sum_{i=1}^{N} \sum_{j=1}^{k} a_{ij} ||\mathbf{x}_i - \boldsymbol{\mu}_j||^2$
- Optimal K-means:
  - $\min_{\mu} \min_{a} F(\mu, a)$

Coordinate descent algorithms

- Want: $\min_a \min_b F(a,b)$

- Coordinate descent:
  - fix a, minimize b
  - fix b, minimize a
  - repeat

- Converges!!!
  - if F is bounded
  - to a (often good) local optimum
    - as we saw in applet (play with it!)

- K-means is a coordinate descent algorithm!

K-means as Co-ordinate Descent

- Optimize objective function:

$$\min_{\boldsymbol{\mu}_1,\ldots,\boldsymbol{\mu}_k} \min_{\boldsymbol{a}_1,\ldots,\boldsymbol{a}_N} F(\boldsymbol{\mu}, \boldsymbol{a}) = \min_{\boldsymbol{\mu}_1,\ldots,\boldsymbol{\mu}_k} \min_{\boldsymbol{a}_1,\ldots,\boldsymbol{a}_N} \sum_{i=1}^{N} \sum_{j=1}^{k} a_{ij} ||\mathbf{x}_i - \boldsymbol{\mu}_j||^2$$

- Fix $\boldsymbol{\mu}$, optimize a (or C)

K-means as Co-ordinate Descent

- Optimize objective function:

$$\min_{\boldsymbol{\mu}_1,\ldots,\boldsymbol{\mu}_k} \min_{\boldsymbol{a}_1,\ldots,\boldsymbol{a}_N} F(\boldsymbol{\mu},\boldsymbol{a}) = \min_{\boldsymbol{\mu}_1,\ldots,\boldsymbol{\mu}_k} \min_{\boldsymbol{a}_1,\ldots,\boldsymbol{a}_N} \sum_{i=1}^{N} \sum_{j=1}^{k} a_{ij} ||\mathbf{x}_i - \boldsymbol{\mu}_j||^2$$

- Fix a (or C), optimize $\boldsymbol{\mu}$

One important use of K-means

- Bag-of-word models in computer vision

Bag of Words model

the world of TOTAL

- All About The Company
- Global Activities
- Corporate Structure
- TOTAL's Story
- Upstream Strategy
- Downstream Strategy
- Chemicals Strategy
- TOTAL Foundation
- Homepage

all about the **company**

Our energy exploration, production, and distribution operations span the globe, with activities in more than 100 countries.

At TOTAL, we draw our greatest strength from our fast-growing oil and gas reserves. Our strategic emphasis on natural gas provides a strong position in a rapidly expanding market.

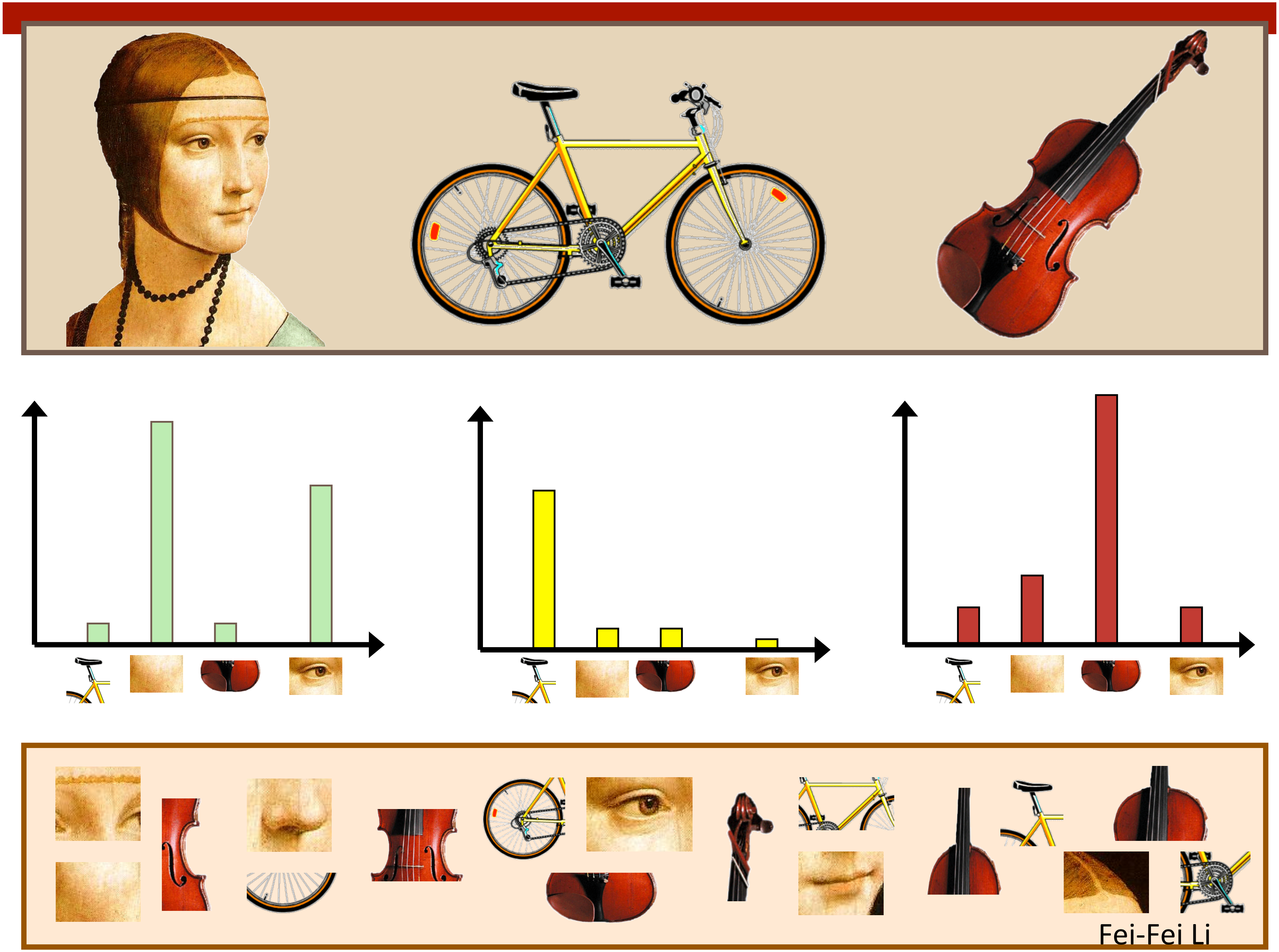
Our expanding refining and marketing operations in Asia and the Mediterranean Rim complement already solid positions in Europe, Africa, and the U.S.

Our growing specialty chemicals sector adds balance and profit to the core energy business.

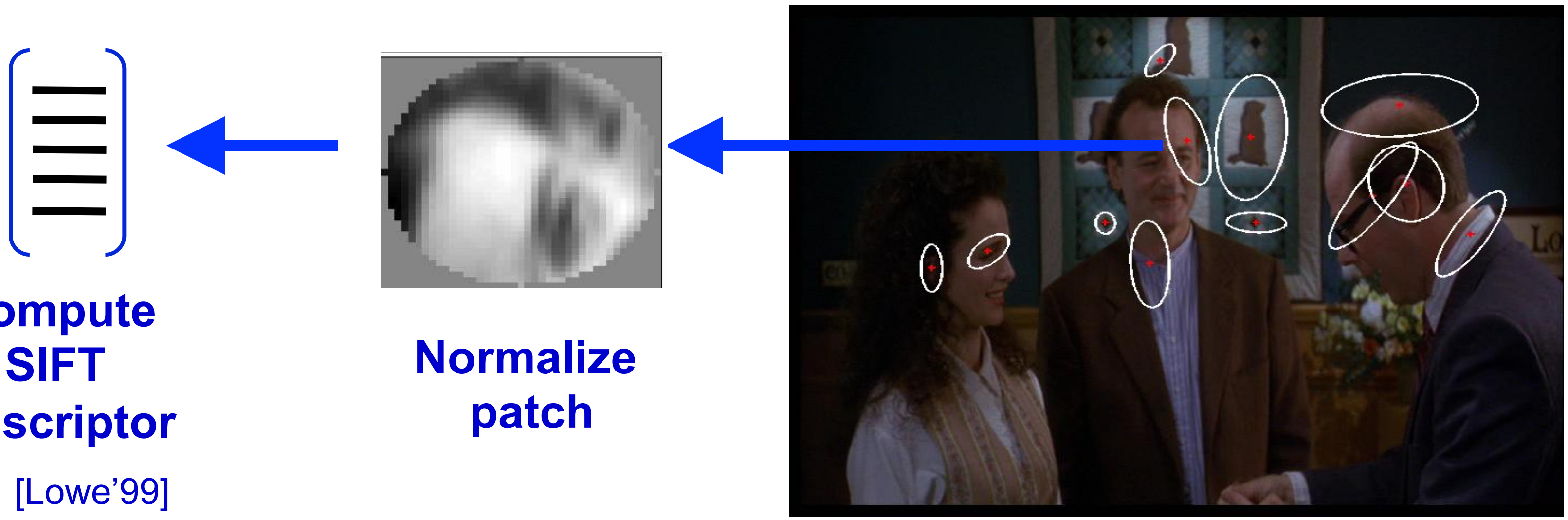
aardvark	0
about	2
all	2
Africa	1
apple	0
anxious	0
...	
gas	1
...	
oil	1
…	
Zaire	0

Object → **Bag of ‘words’**

Fei-Fei Li


Fei-Fei Li

Interest Point Features



Compute SIFT descriptor

[Lowe'99]

Normalize patch

Detect patches

[Mikojaczyk and Schmid '02]

[Matas et al. '02]

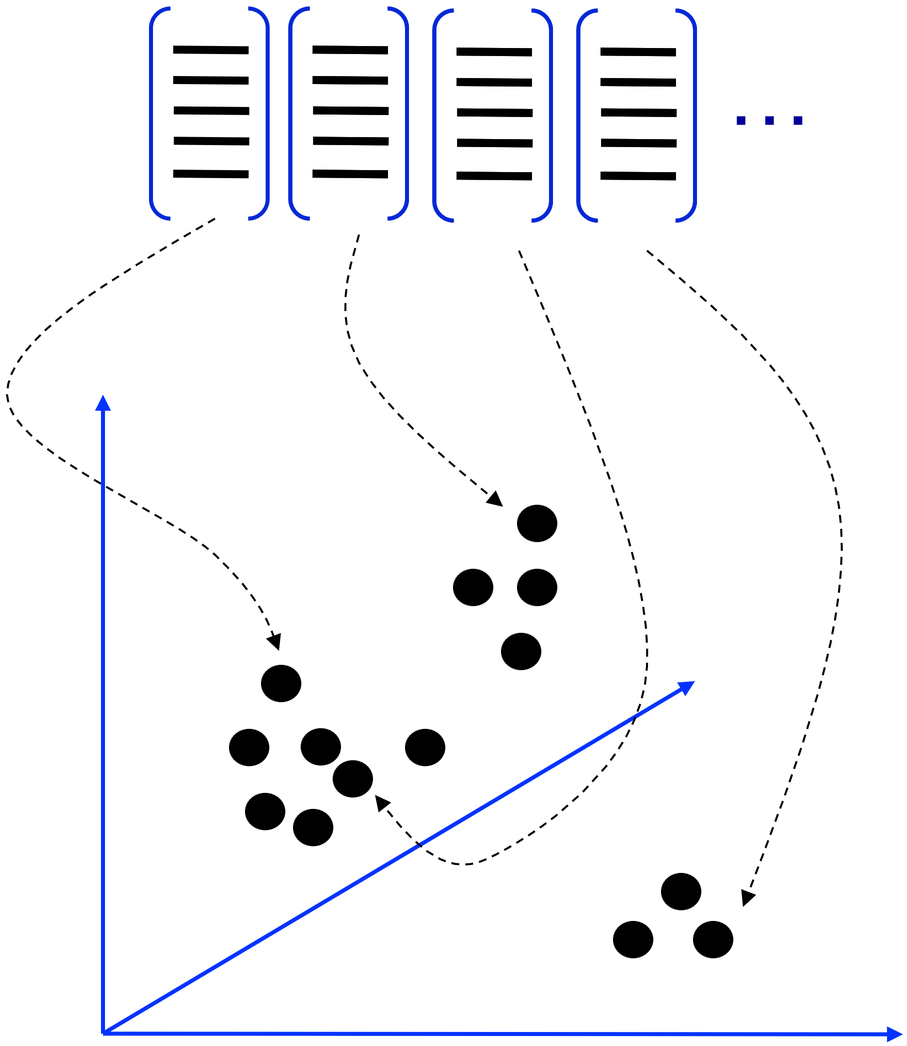
[Sivic et al. '03]

Slide credit: Josef Sivic

Patch Features

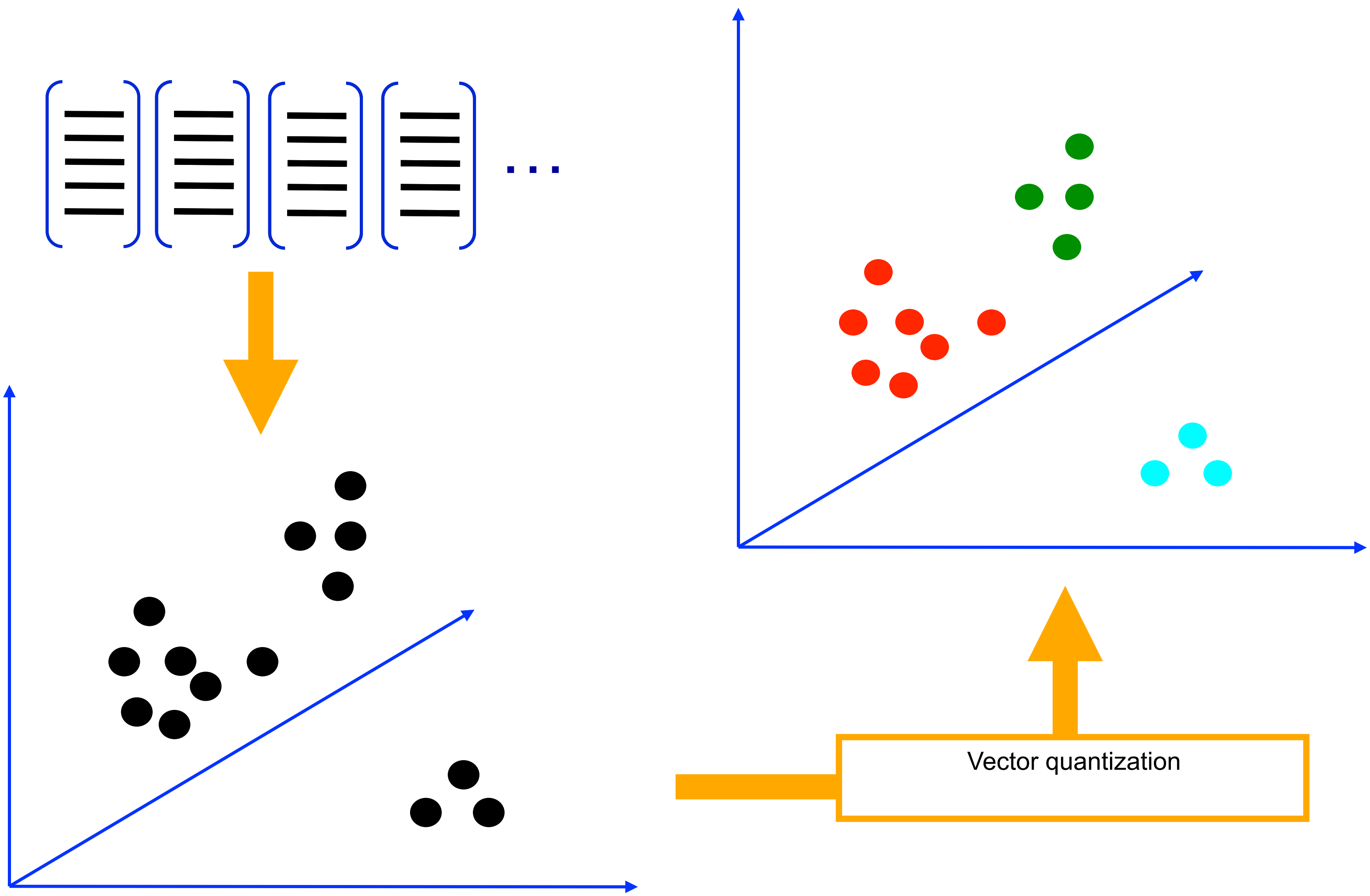
Slide credit: Josef Sivic

dictionary formation



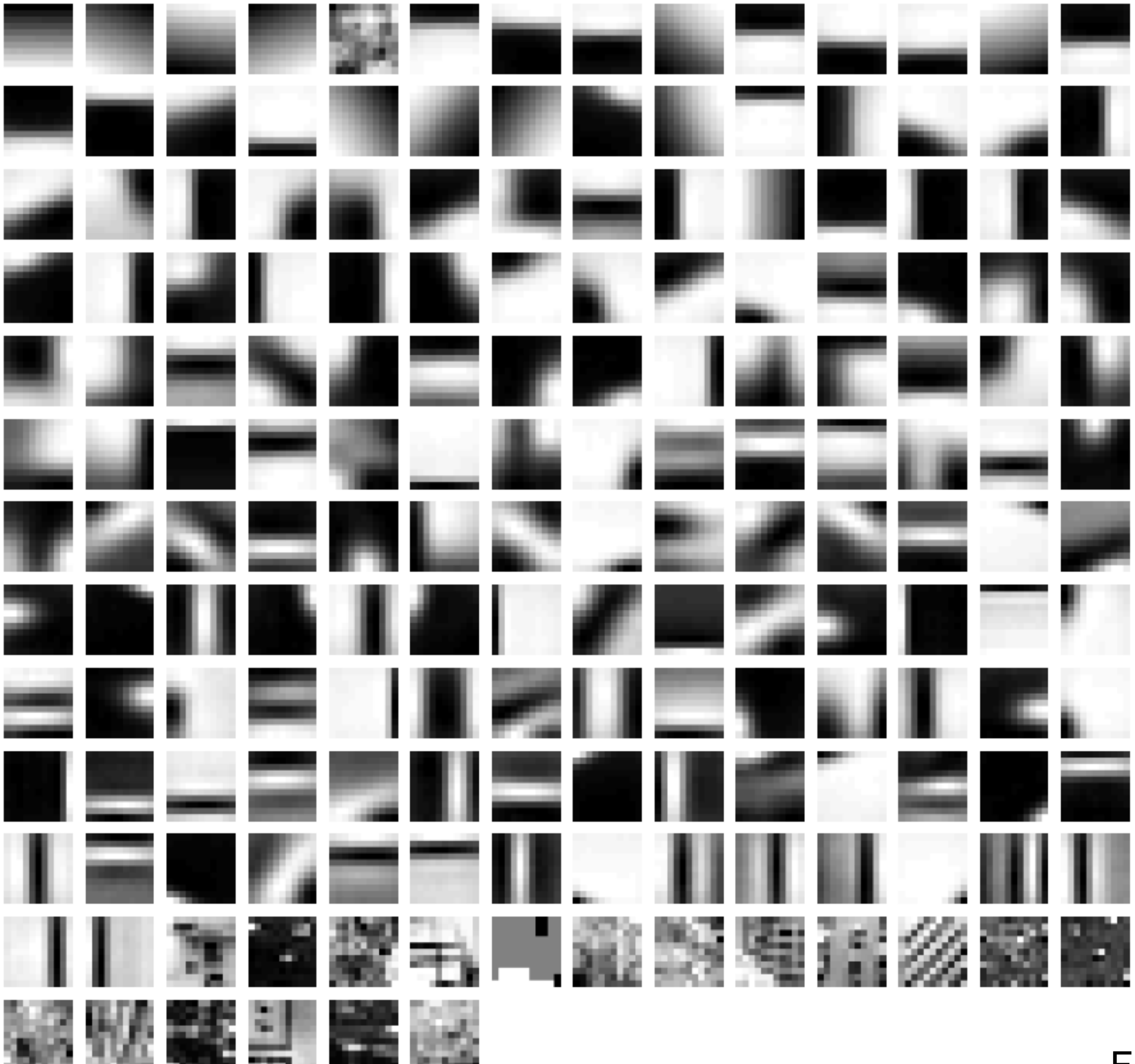
Slide credit: Josef Sivic

Clustering (usually k-means)



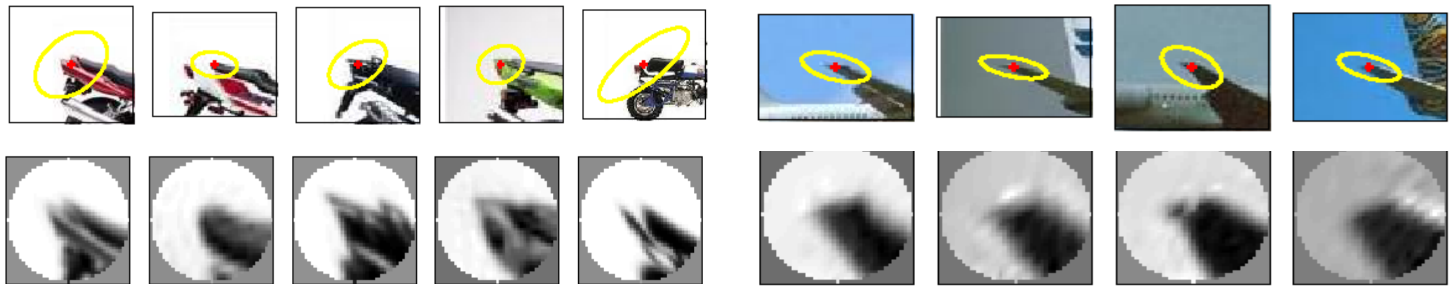
Slide credit: Josef Sivic

Clustered Image Patches



Fei-Fei et al. 2005

Visual synonyms and polysemy

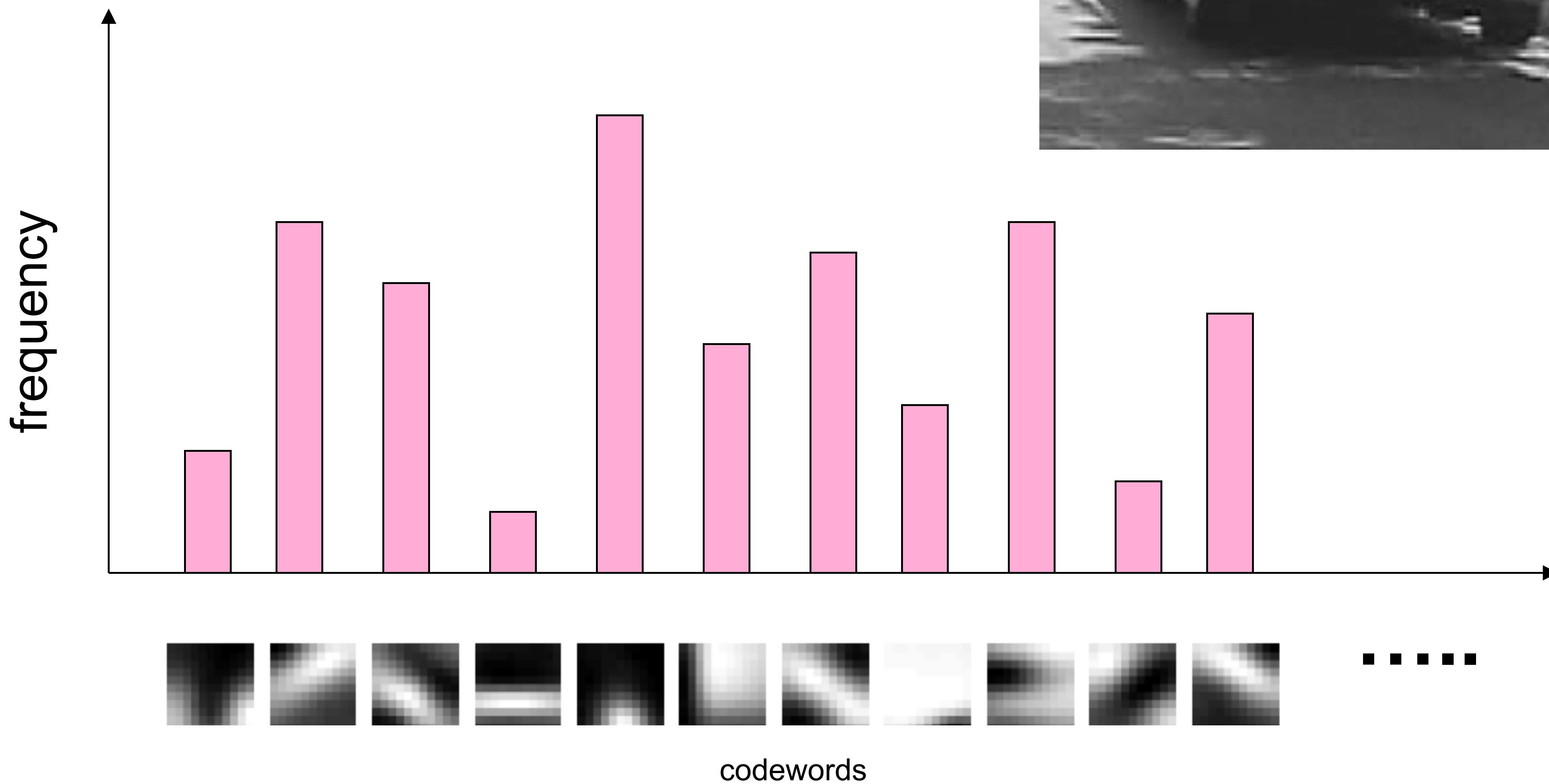


Visual Polysemy. Single visual word occurring on different (but locally similar) parts on different object categories.

Visual Synonyms. Two different visual words representing a similar part of an object (wheel of a motorbike).

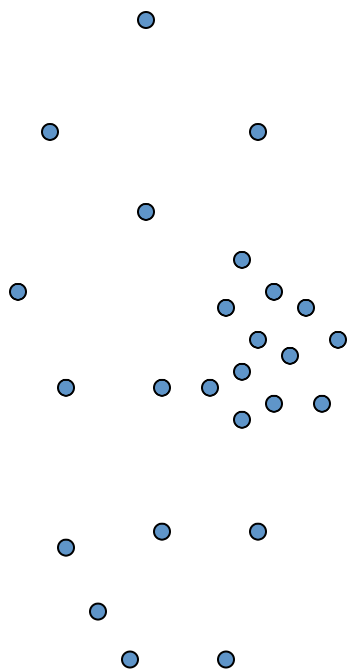
Andrew Zisserman

Image representation



Fei-Fei Li

(One) bad case for k-means



- Clusters may overlap
- Some clusters may be "wider" than others

- GMM to the rescue!

GMM

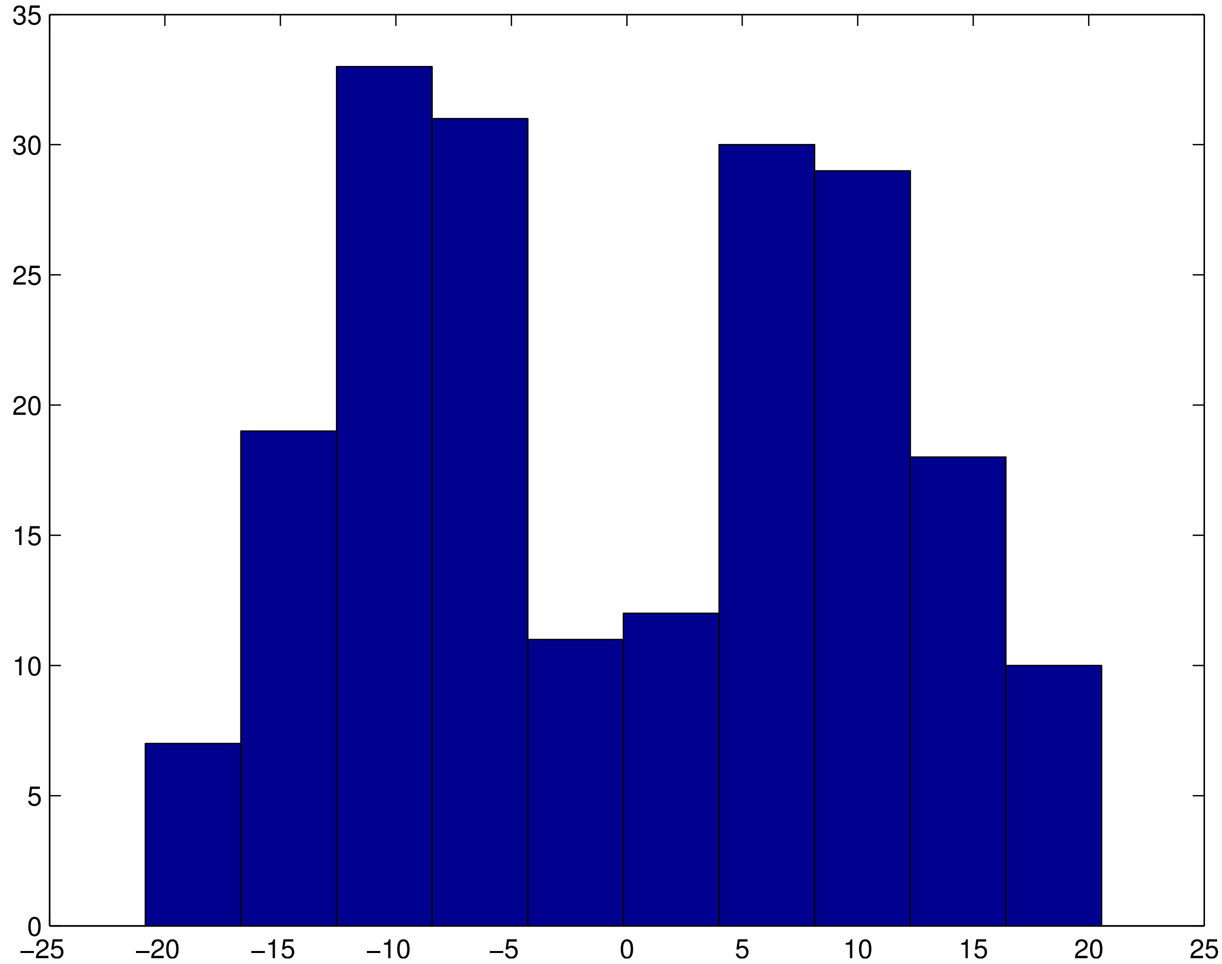
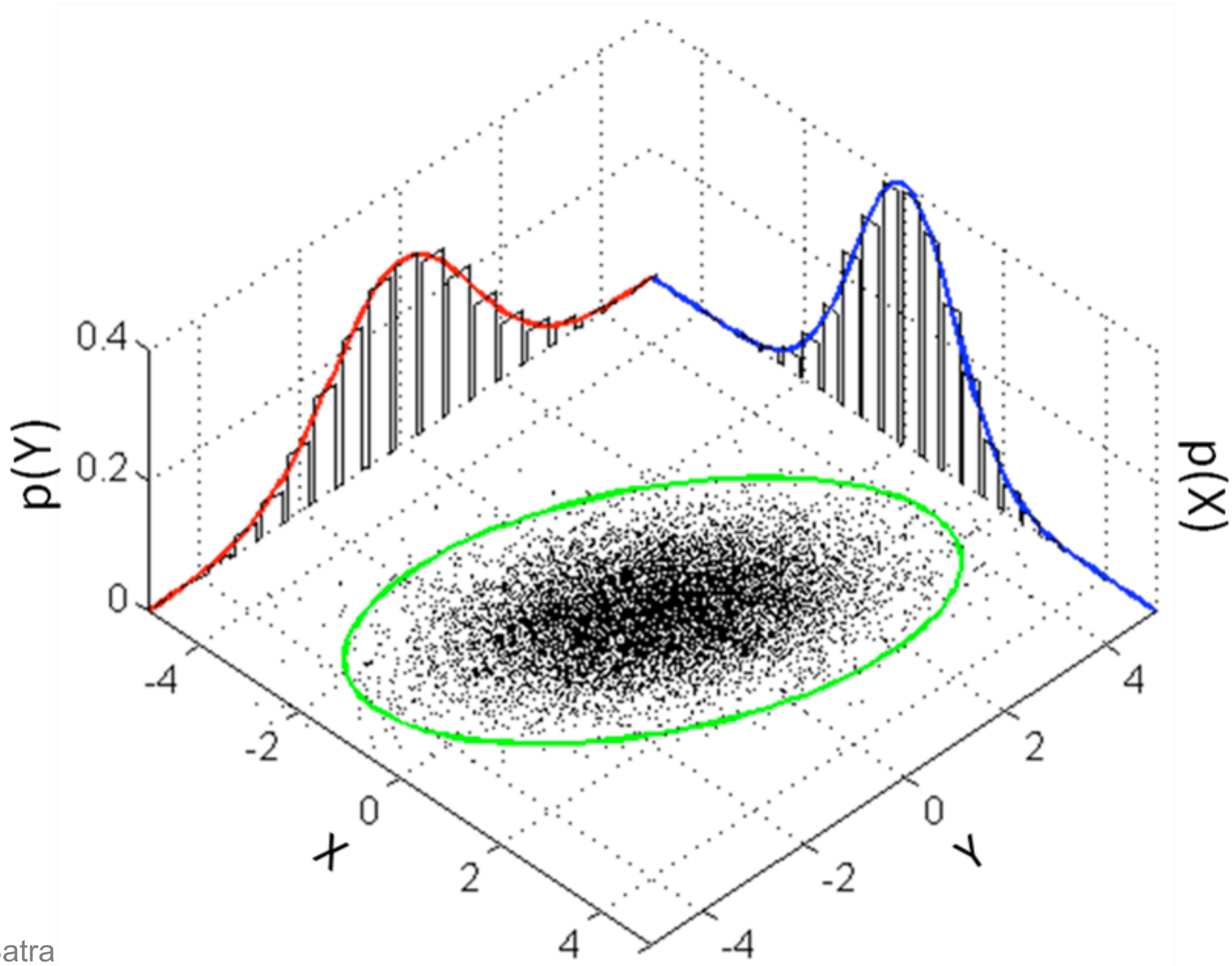
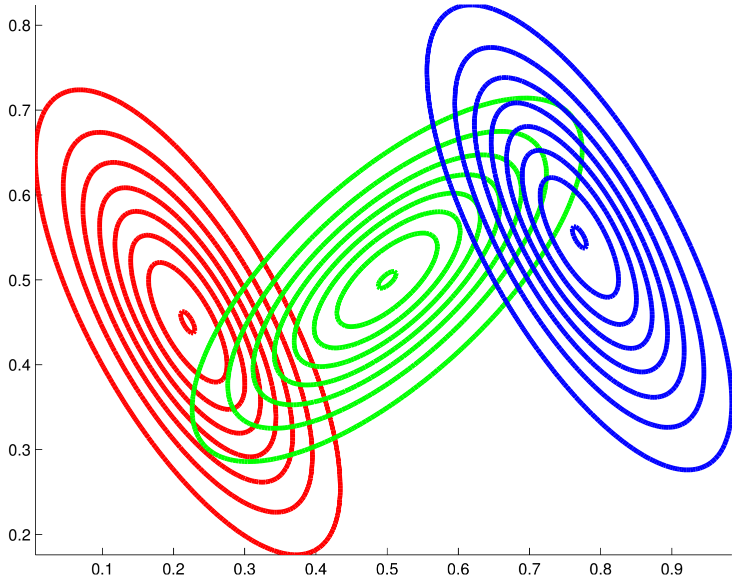


Figure Credit: Kevin Murphy

Recall Multi-variate Gaussians



GMM



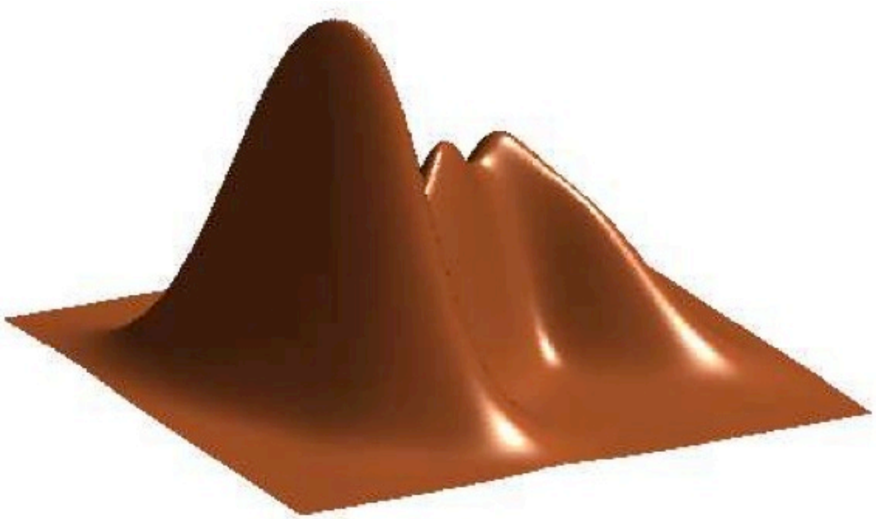


Figure Credit: Kevin Murphy

Hidden Data Causes Problems #1

- Fully Observed (Log) Likelihood factorizes
- Marginal (Log) Likelihood doesn't factorize
- All parameters coupled!

GMM vs Gaussian Joint Bayes Classifier

- On Board
  - Observed Y vs Unobserved Z
  - Likelihood vs Marginal Likelihood

Hidden Data Causes Problems #2

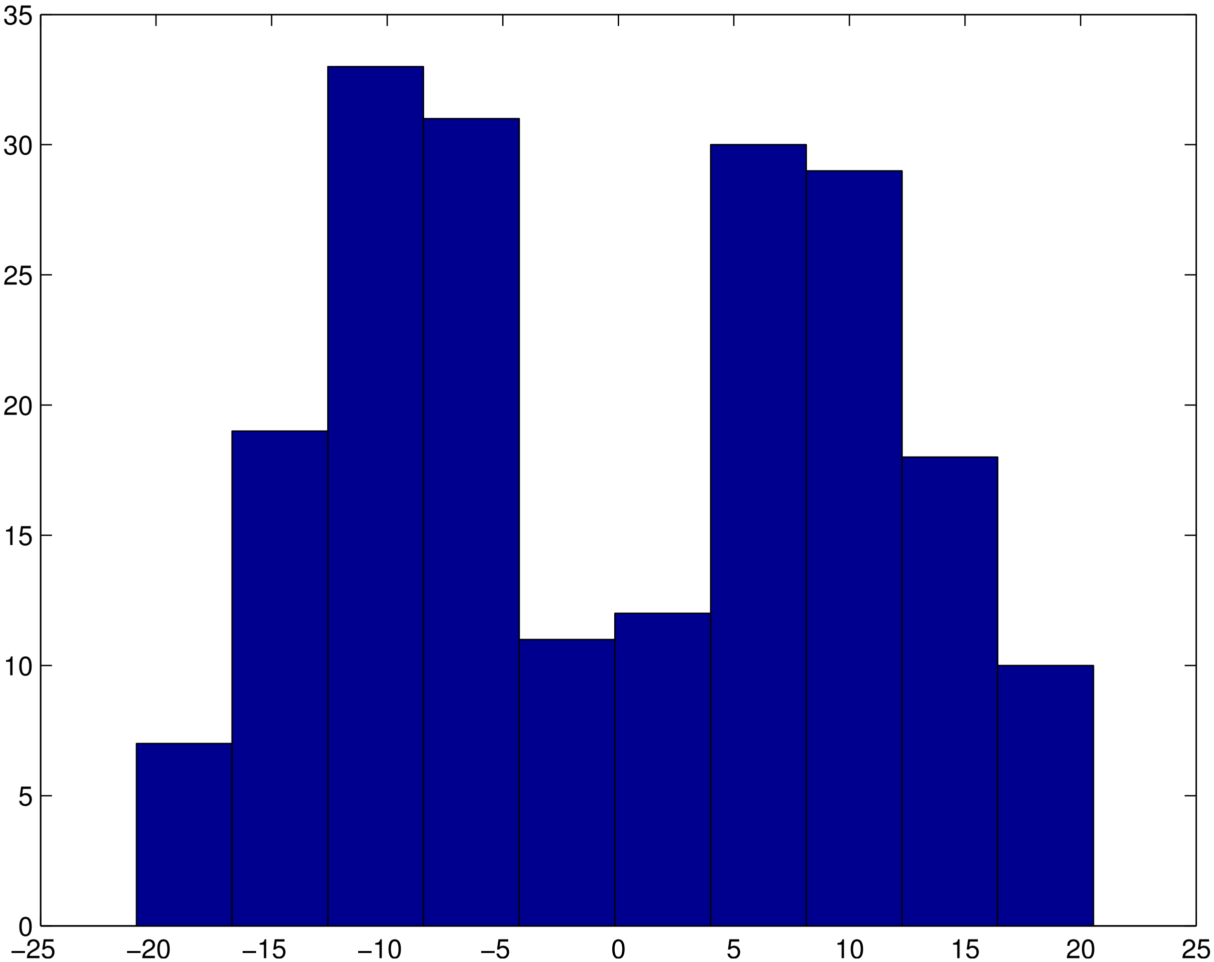
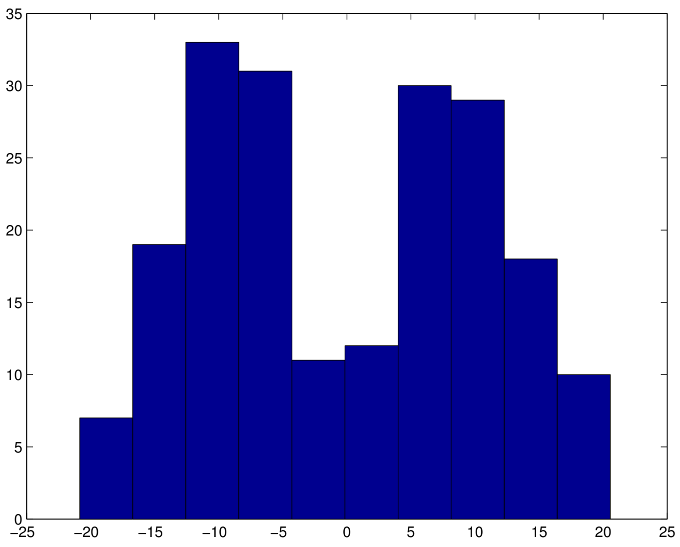
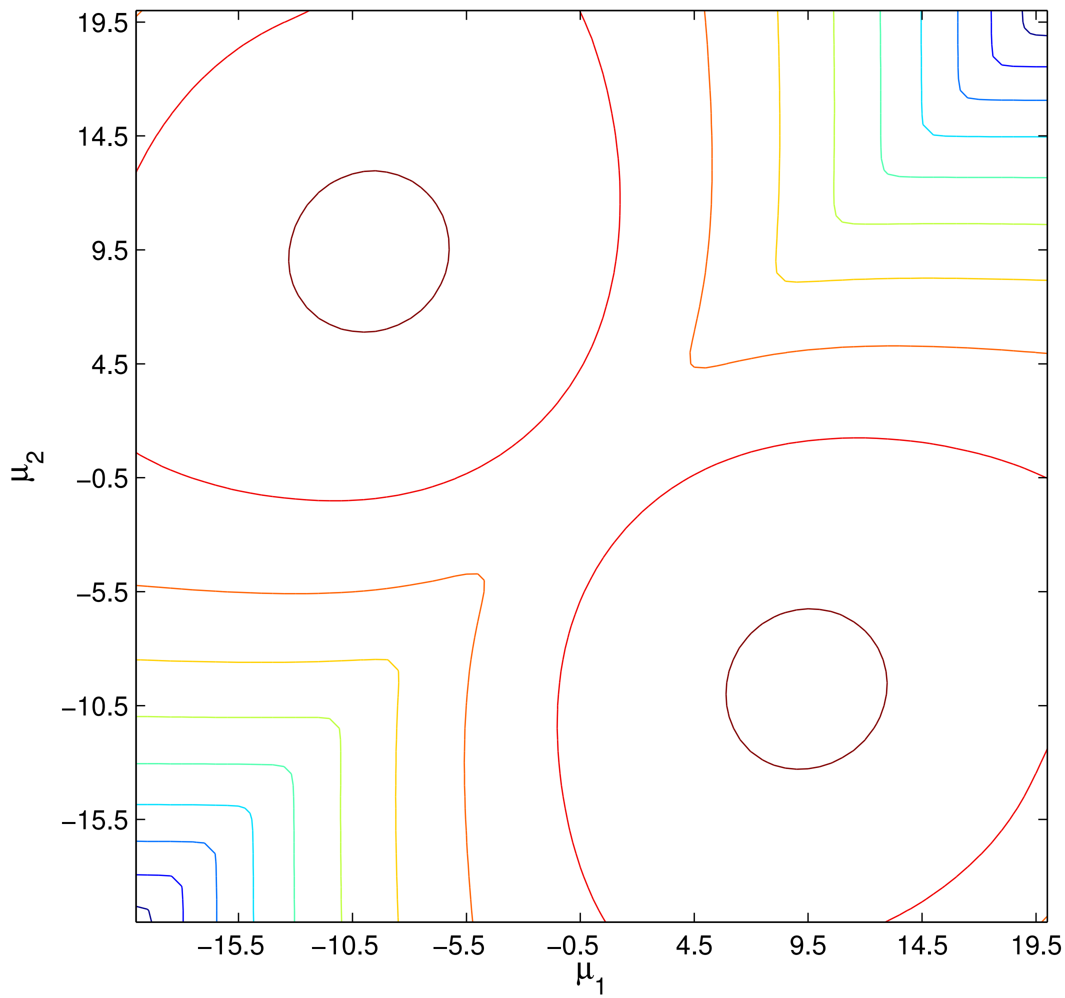


Figure Credit: Kevin Murphy

Hidden Data Causes Problems #2

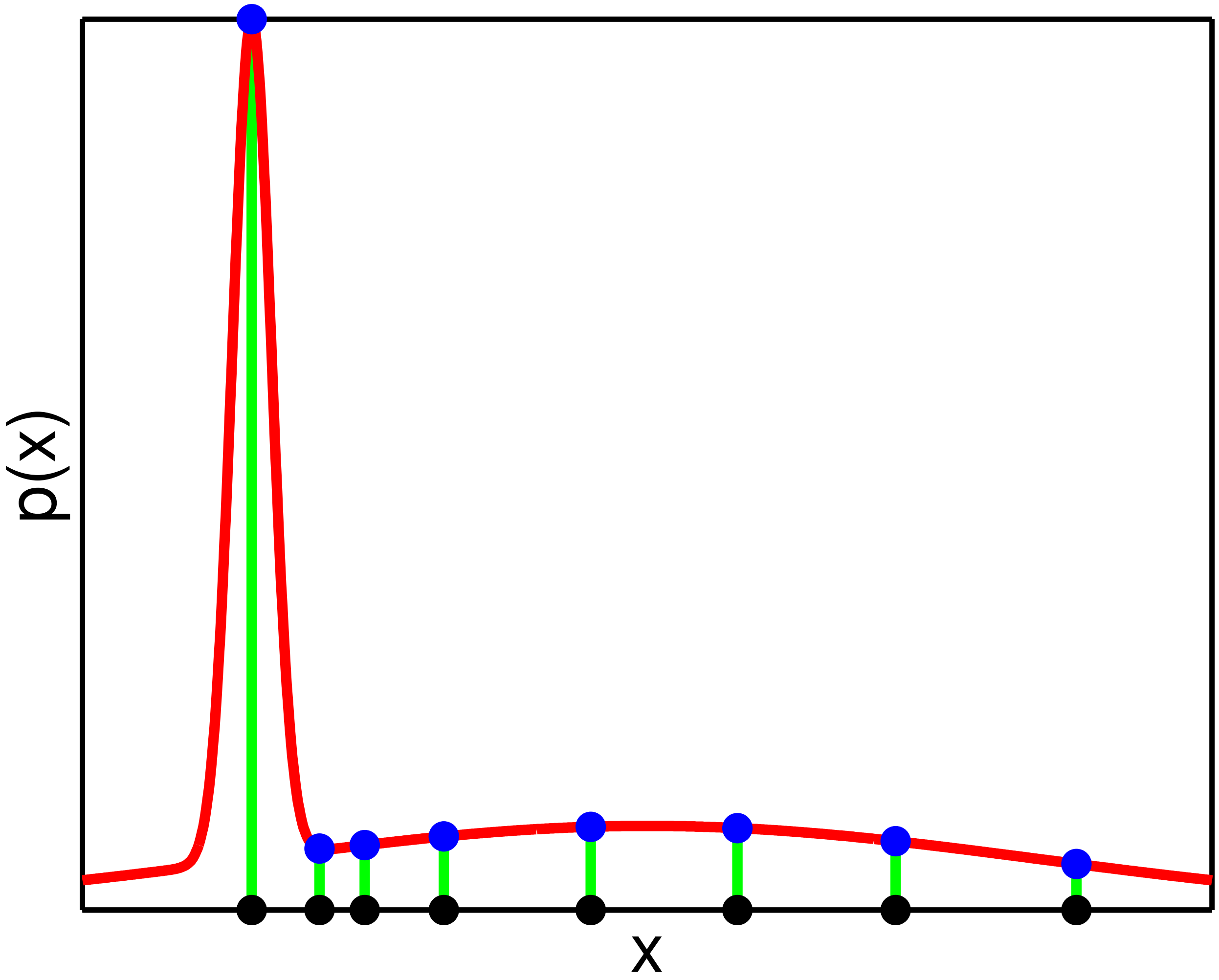
- Identifiability





Hidden Data Causes Problems #3

- Likelihood has singularities if one Gaussian "collapses"



Special case: spherical Gaussians and hard assignments

- If P(X|Z=k) is spherical, with same σ for all classes:

$$P(\mathbf{x}_i \mid z = j) \propto \exp\left[-\frac{1}{2\sigma^2}\left\|\mathbf{x}_i - \mu_j\right\|^2\right]$$

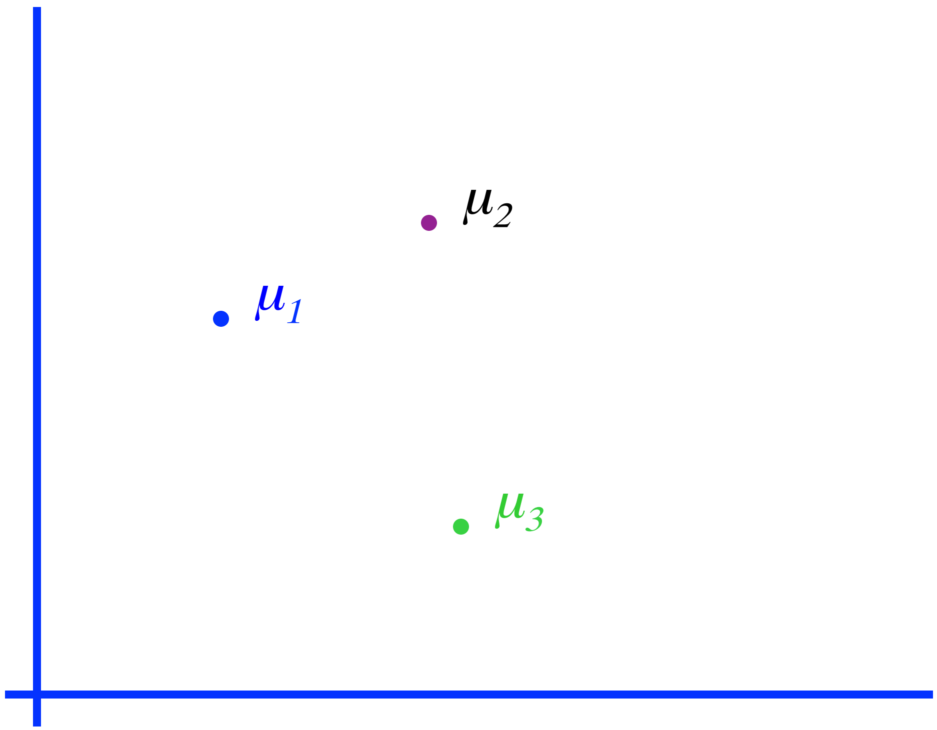
- If each x_i belongs to one class C(i) (hard assignment), marginal likelihood:

$$\prod_{i=1}^{N}\sum_{j=1}^{k} P(\mathbf{x}_i, y = j) \propto \prod_{i=1}^{N}\exp\left[-\frac{1}{2\sigma^2}\left\|\mathbf{x}_i - \mu_{C(i)}\right\|^2\right]$$

- M(M)LE same as K-means!!!

The K-means GMM assumption

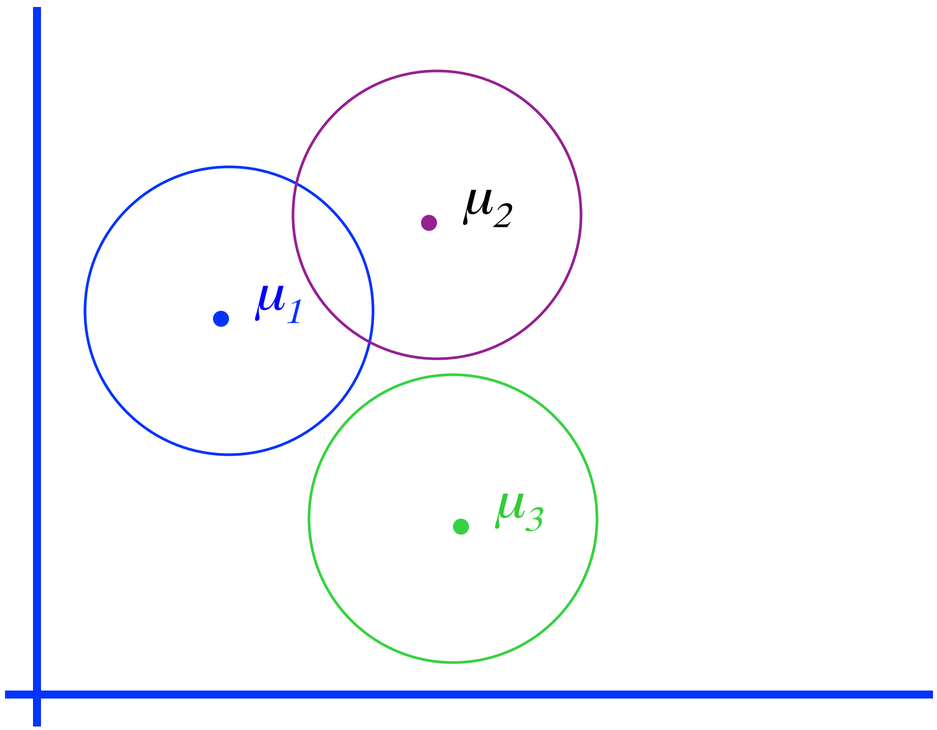
- There are k components
- Component *i* has an associated mean vector μ_ι



The K-means GMM assumption

- There are k components
- Component *i* has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean m_i and covariance matrix $\sigma^2 I$

Each data point is generated according to the following recipe:



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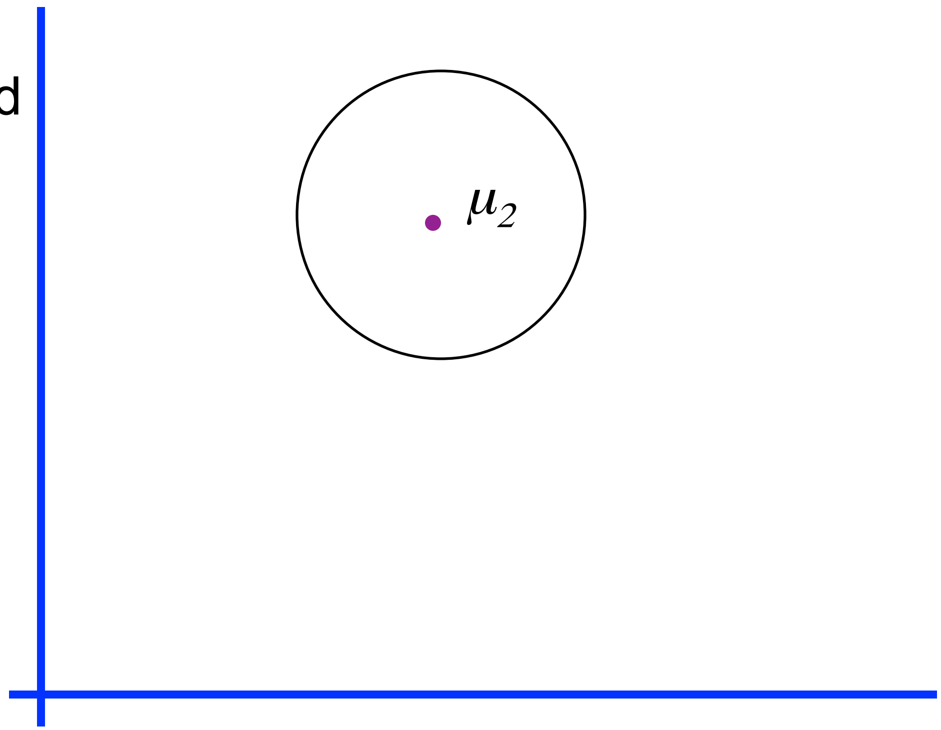
Each data point is generated according to the following recipe:

1. Pick a component at random: Choose component i with probability $P(y=i)$



The K-means GMM assumption

- There are k components
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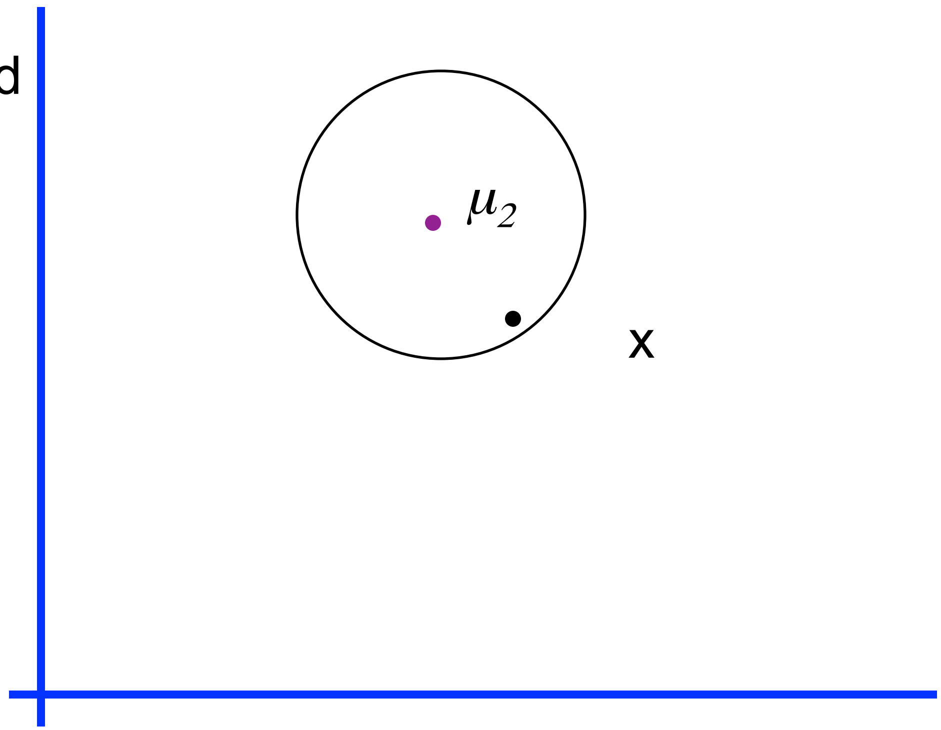
- Each component generates data from a Gaussian with mean m_i and covariance matrix $\sigma^2 \boldsymbol{I}$

Each data point is generated according to the following recipe:

1. Pick a component at random: Choose component i with probability *P(y=i)*
2. Datapoint $\sim N(\mu_i, \sigma^2 \boldsymbol{I})$

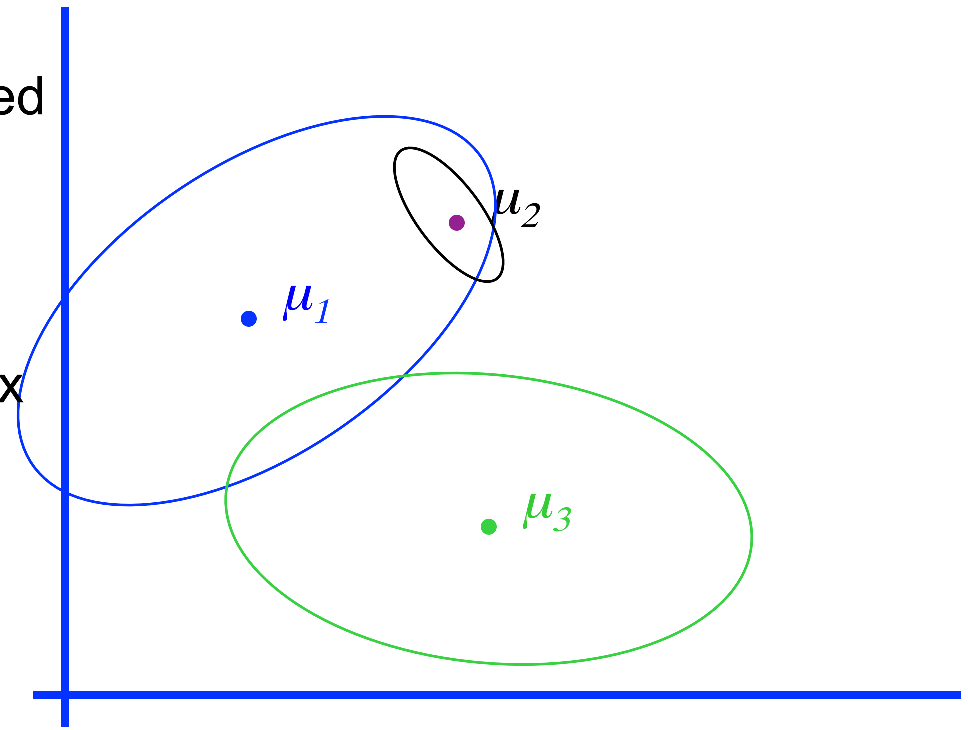


The General GMM assumption

- There are k components
- Component *i* has an associated mean vector m_i
- Each component generates data from a Gaussian with mean m_i and covariance matrix Σ_i

Each data point is generated according to the following recipe:

1. Pick a component at random: Choose component i with probability *P(y=i)*
2. Datapoint ~ N(m_i, Σ_i)



K-means vs GMM

- K-Means
  - http://home.deib.polimi.it/matteucc/Clustering/tutorial_html/AppletKM.html

- GMM
  - http://www.socr.ucla.edu/applets.dir/mixtureem.html