Unsupervised Learning: K-Means & PCA

Unsupervised Learning

- Supervised learning used labeled data pairs $(\mathbf{x}, \mathrm{y})$ to learn a function $f : \mathrm{X} \rightarrow \mathrm{Y}$
  - But, what if we don't have labels?

- No labels = **unsupervised learning**
- Only some points are labeled = **semi-supervised learning**
  - Labels may be expensive to obtain, so we only get a few

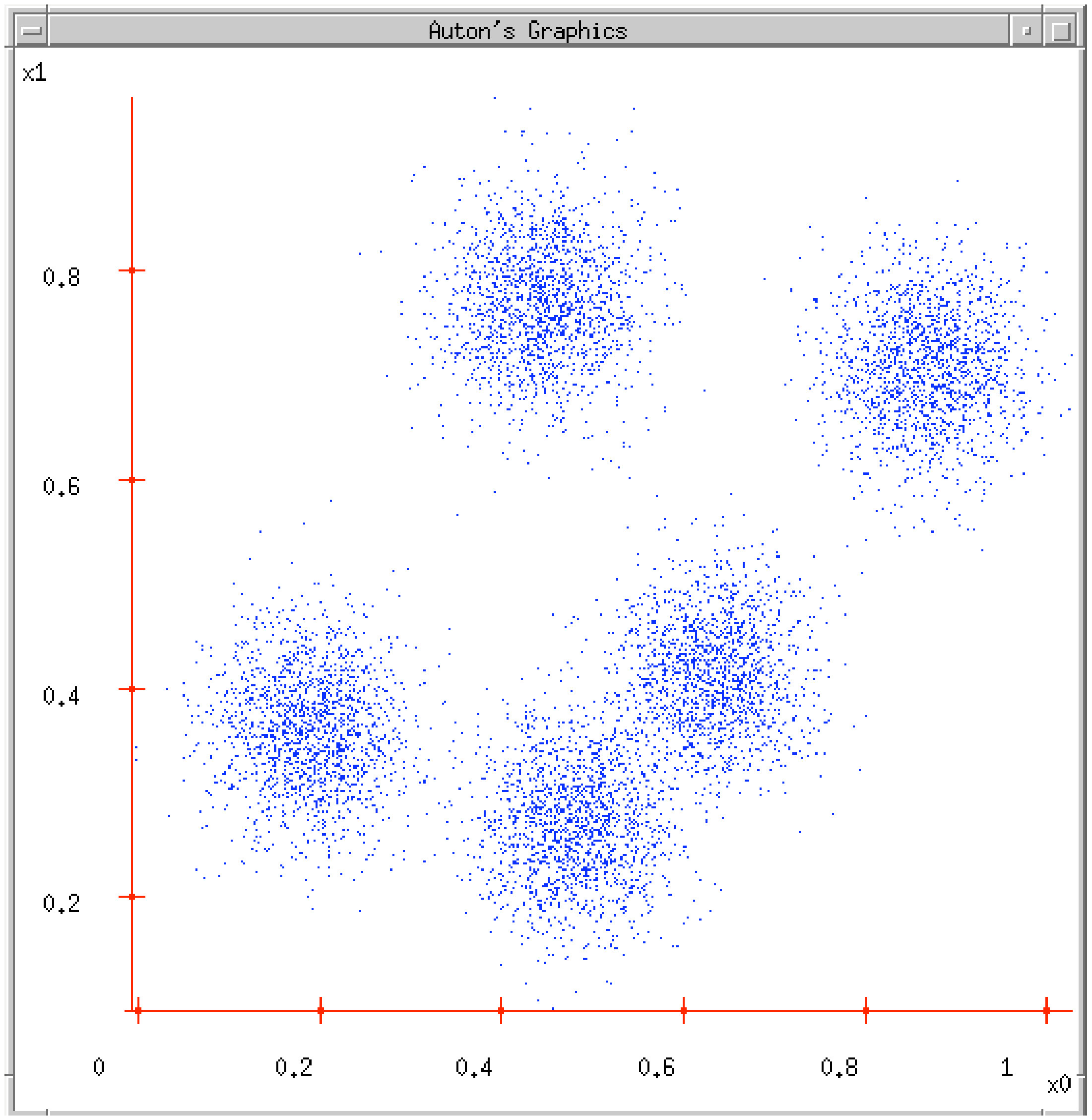
- **Clustering** is the unsupervised grouping of data points. It can be used for **knowledge discovery**.

K-Means Clustering

Some material adapted from slides by Andrew Moore, CMU.

Visit http://www.autonlab.org/tutorials/ for
Andrew’s repository of Data Mining tutorials.

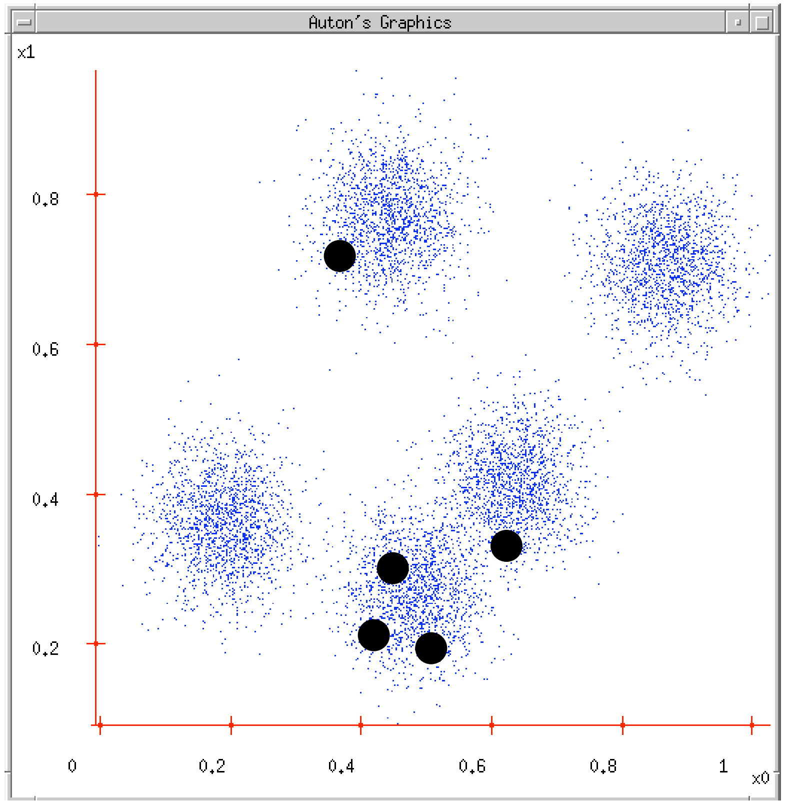
Clustering Data



K-Means Clustering

K-Means (k , X)

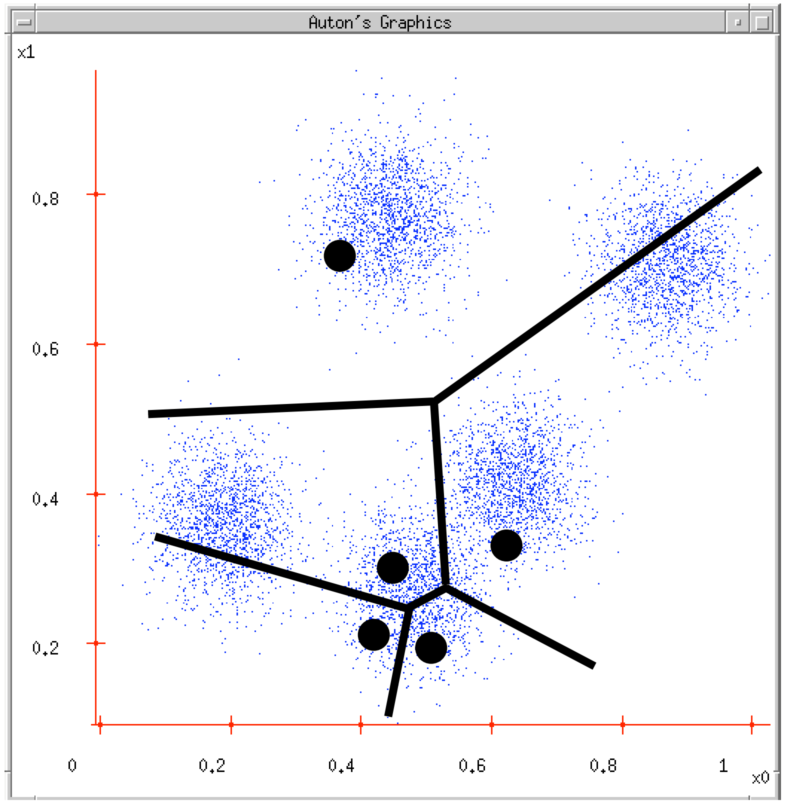
- Randomly choose k cluster center locations (centroids)
- Loop until convergence
  - Assign each point to the cluster of the closest centroid
  - Re-estimate the cluster centroids based on the data assigned to each cluster



K-Means Clustering

K-Means (k , X)

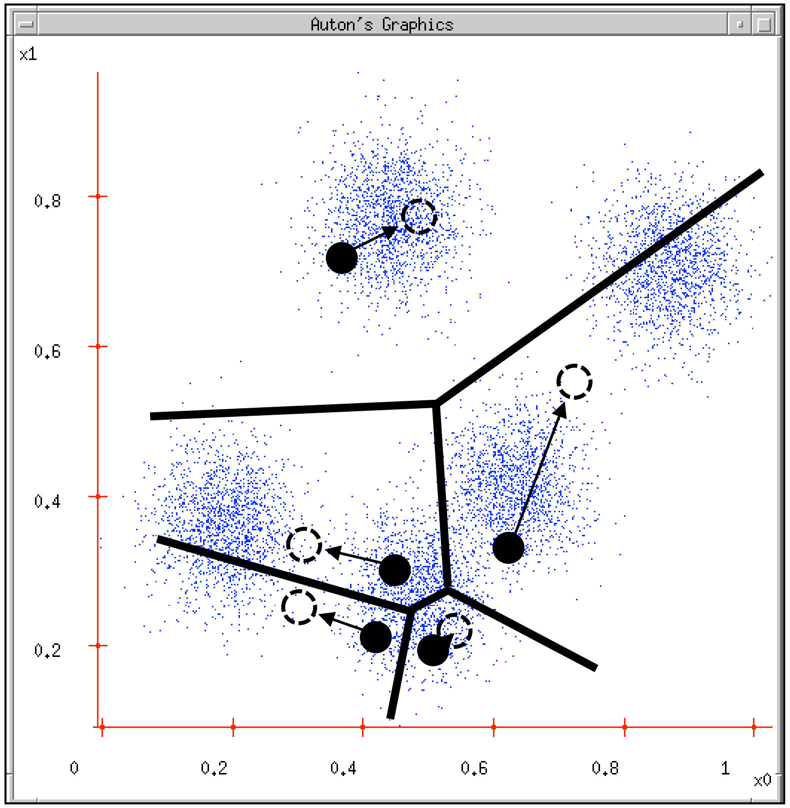
- Randomly choose k cluster center locations (centroids)
- Loop until convergence
  - Assign each point to the cluster of the closest centroid
  - Re-estimate the cluster centroids based on the data assigned to each cluster



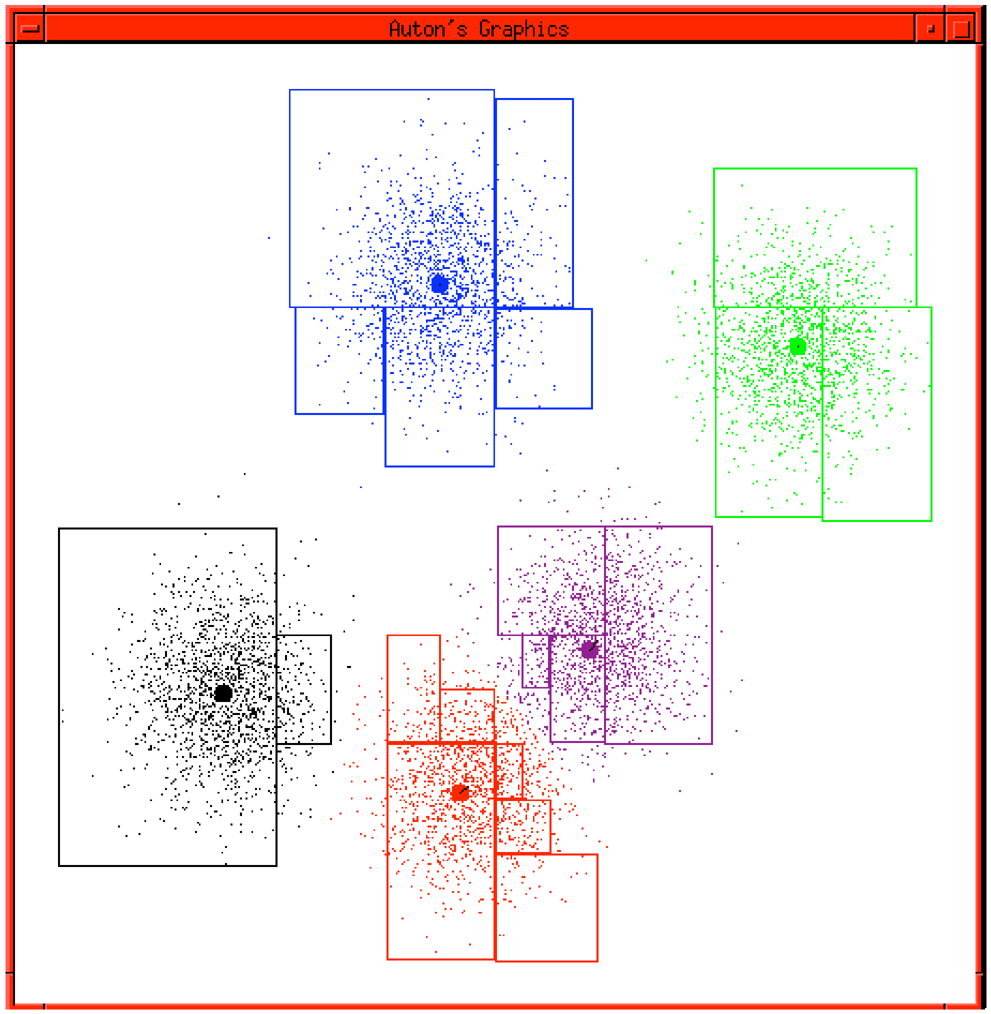
K-Means Clustering

K-Means (k , X)

- Randomly choose k cluster center locations (centroids)
- Loop until convergence
  - Assign each point to the cluster of the closest centroid
  - Re-estimate the cluster centroids based on the data assigned to each cluster



K-Means Animation



Example generated by Andrew Moore using Dan Pelleg's super-duper fast K-means system:

Dan Pelleg and Andrew Moore. Accelerating Exact k-means Algorithms with Geometric Reasoning. Proc. Conference on Knowledge Discovery in Databases 1999.

K-Means Objective Function

- K-means finds a local optimum of the following objective function:

$$\arg\min_{\boldsymbol{\mathcal{S}}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in \mathcal{S}_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|_2^2$$

where $\boldsymbol{\mathcal{S}} = \{\mathcal{S}_1, \ldots, \mathcal{S}_k\}$ is a partitioning over $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ s.t. $X = \bigcup_{i=1}^{k} \mathcal{S}_i$ and $\boldsymbol{\mu}_i = \text{mean}(\mathcal{S}_i)$

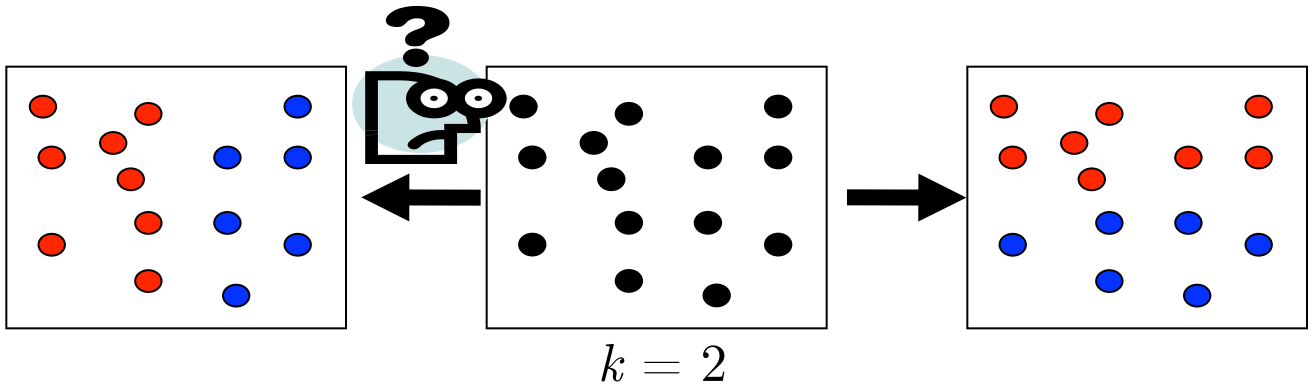
Problems with K-Means

- ***Very*** sensitive to the initial points
  - Do many runs of K-Means, each with different initial centroids
  - Seed the centroids using a better method than randomly choosing the centroids
    - e.g., Farthest-first sampling

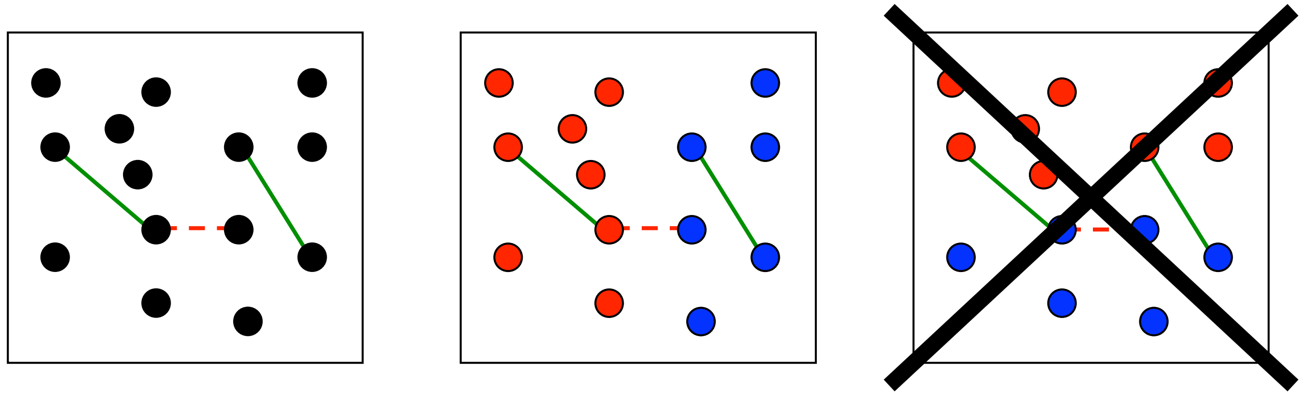
- Must manually choose k
  - Learn the optimal k for the clustering
    - Note that this requires a performance measure

Problems with K-Means

- How do you tell it which clustering you want?



Constrained clustering techniques (semi-supervised)

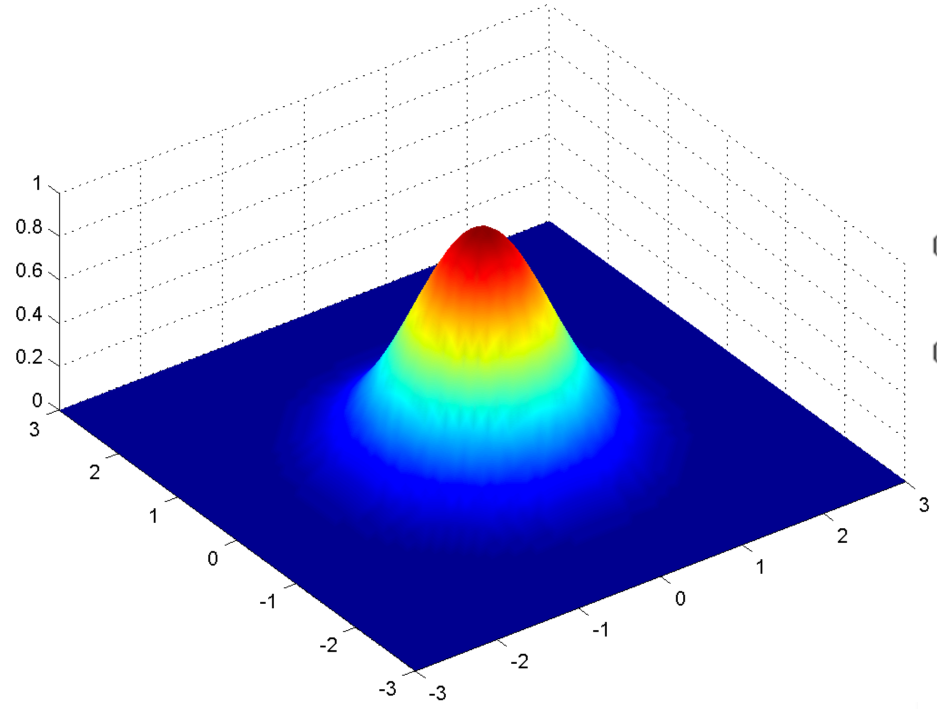


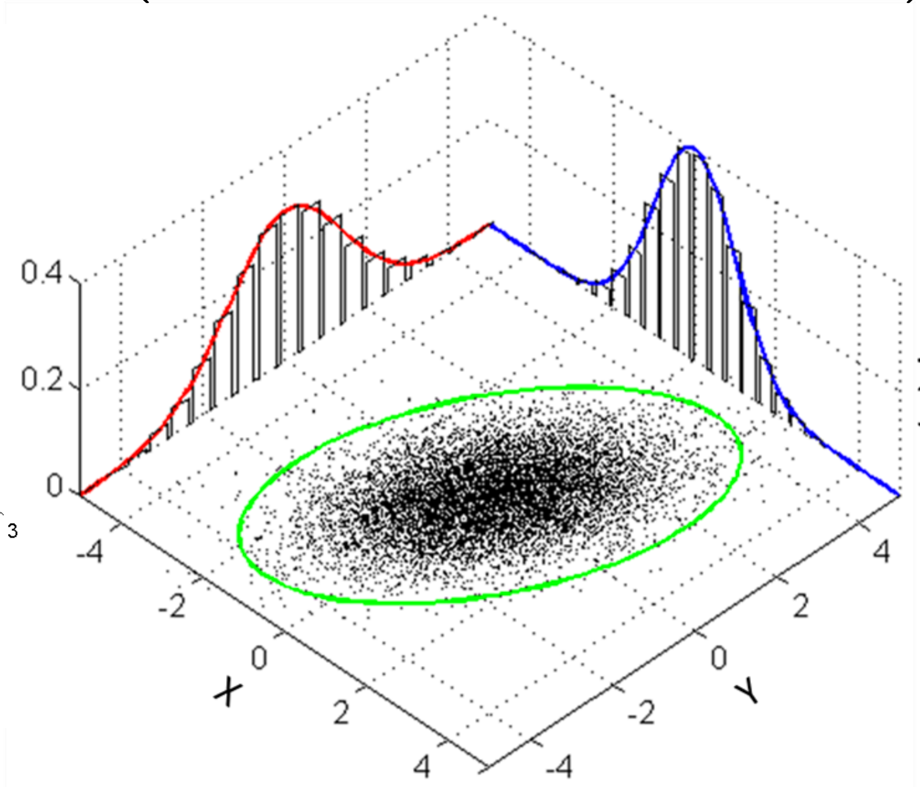
Same-cluster constraint
(must-link)
Different-cluster constraint
(cannot-link)

Gaussian Mixture Models

- Recall the Gaussian distribution:

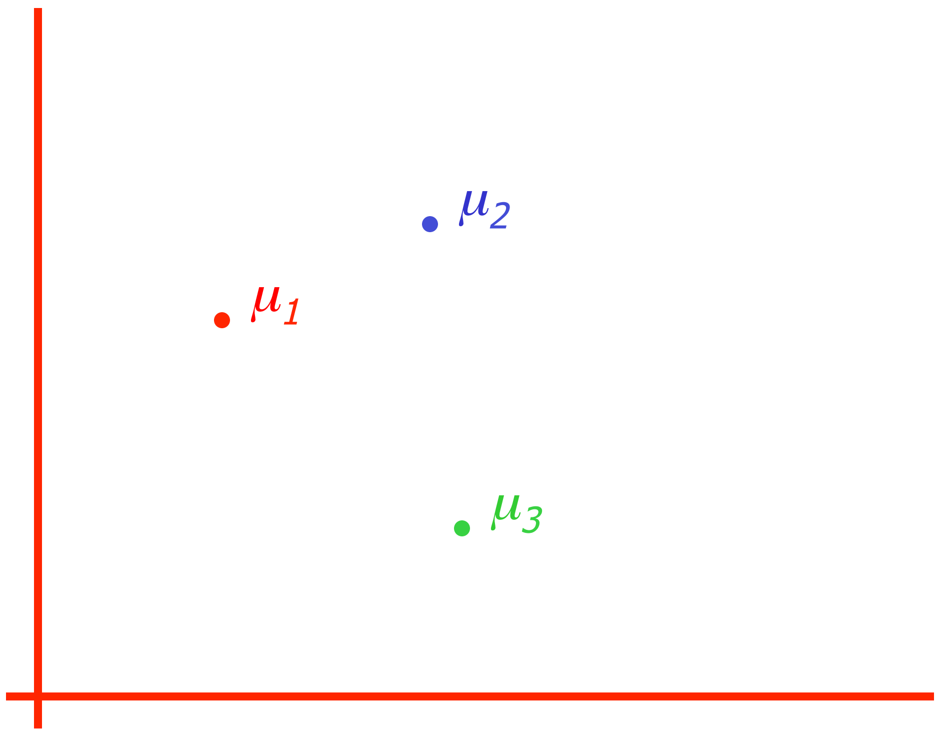
$$P(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$





The GMM assumption

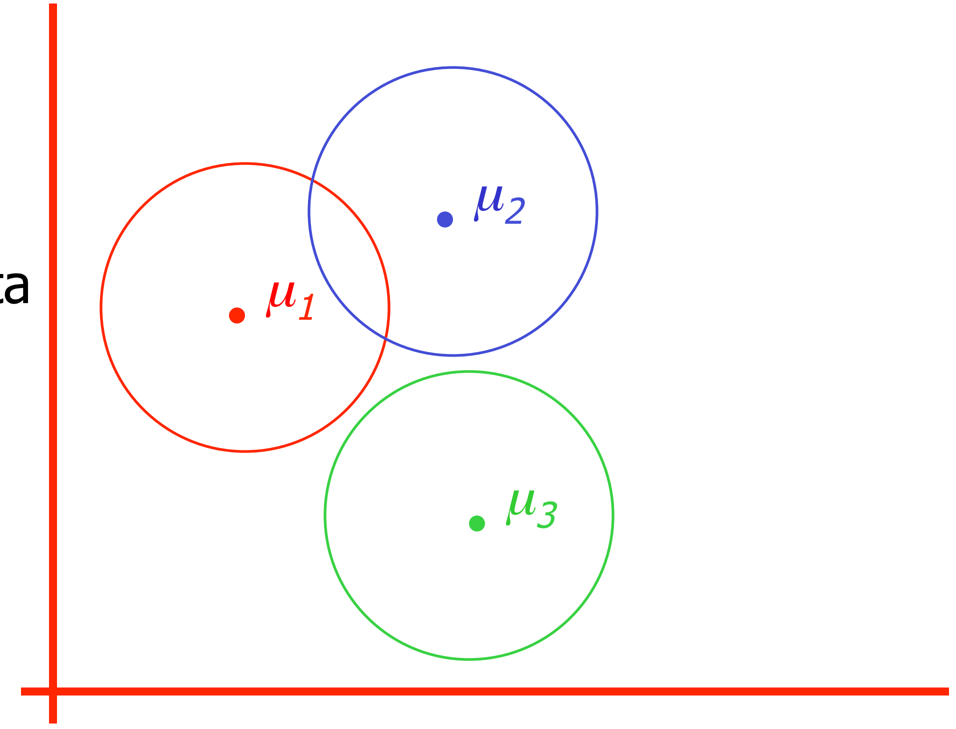
- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i



The GMM assumption

- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean μ_i and covariance matrix $\sigma^2 \boldsymbol{I}$

Assume that each datapoint is generated according to the following recipe:

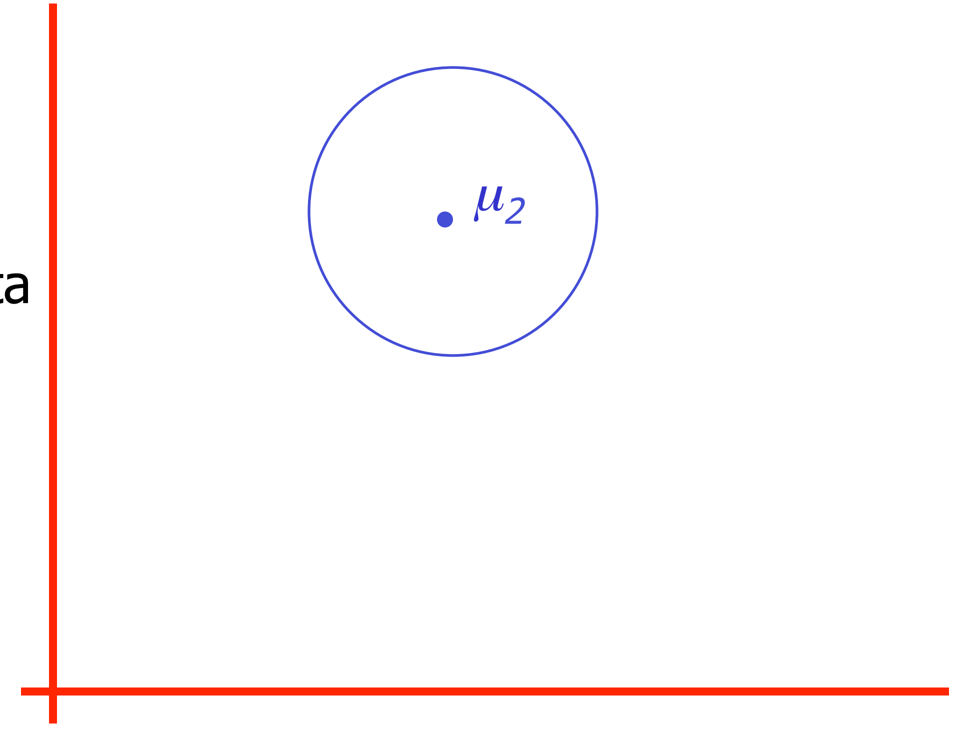


The GMM assumption

- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean μ_i and covariance matrix $\sigma^2\boldsymbol{I}$

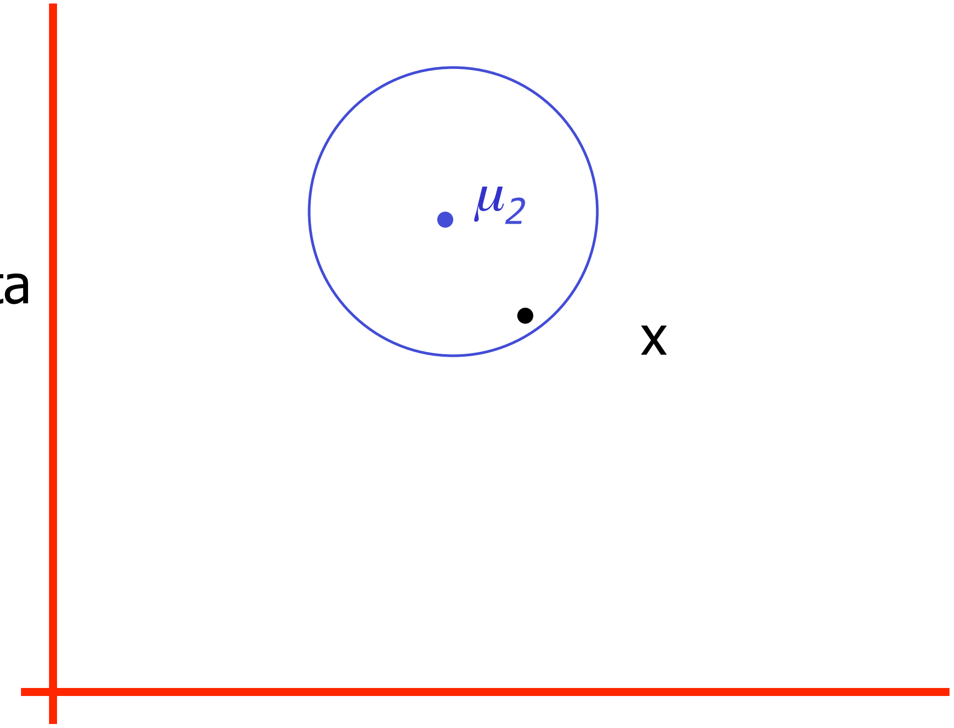
Assume that each datapoint is generated according to the following recipe:

1. Pick a component at random. Choose component i with probability $P(\omega_i)$.



The GMM assumption

- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean μ_i and covariance matrix $\sigma^2\boldsymbol{I}$



Assume that each datapoint is generated according to the following recipe:

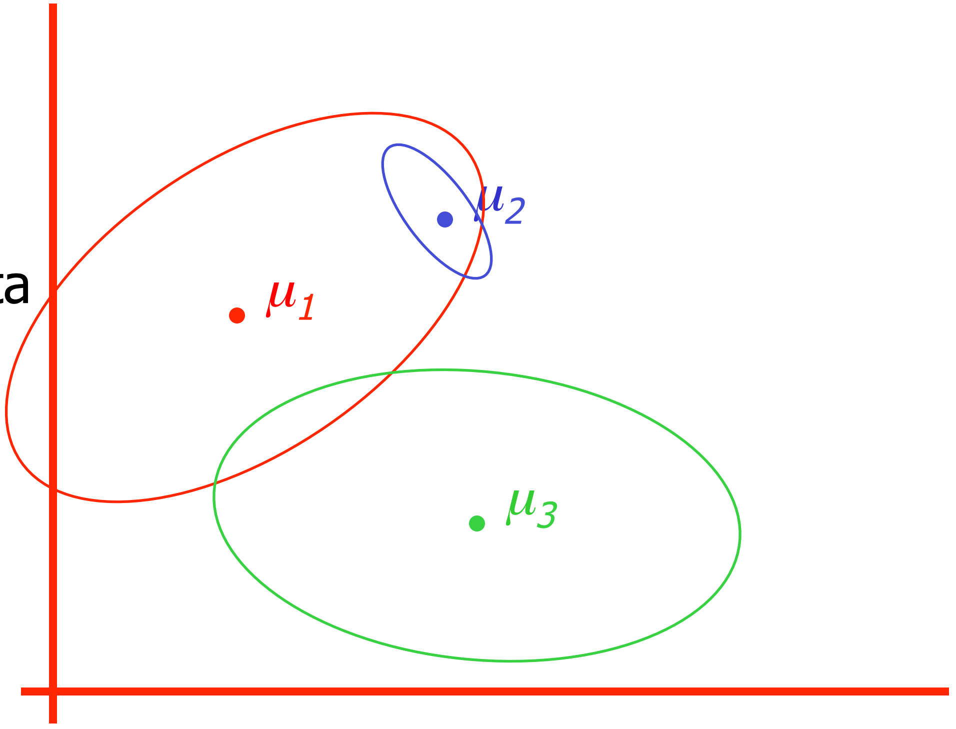
1. Pick a component at random. Choose component i with probability $P(\omega_i)$.
2. Datapoint ~ N(μ_i, $\sigma^2\boldsymbol{I}$)

The General GMM assumption

- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean μ_i and covariance matrix Σ_i

Assume that each datapoint is generated according to the following recipe:

1. Pick a component at random. Choose component i with probability $P(\omega_i)$.
2. Datapoint ~ N(μ_i, Σ_i)



Fitting a Gaussian Mixture Model

(Optional)

Expectation-Maximization for GMMs

Iterate until convergence:

On the *t*' th iteration let our estimates be

$$\lambda_t = \{ \mu_1(t), \mu_2(t) \ldots \mu_c(t) \}$$

E-step: Compute "expected" classes of all datapoints for each class

Just evaluate a Gaussian at x_k

$$\mathrm{P}(w_i | x_k, \lambda_t) = \frac{\mathrm{p}(x_k | w_i, \lambda_t) \mathrm{P}(w_i | \lambda_t)}{\mathrm{p}(x_k | \lambda_t)} = \frac{\mathrm{p}(x_k | w_i, \mu_i(t), \sigma^2 \mathbf{I}) p_i(t)}{\sum_{j=1}^{c} \mathrm{p}(x_k | w_j, \mu_j(t), \sigma^2 \mathbf{I}) p_j(t)}$$

M-step: Estimate **μ** given our data's class membership distributions

$$\mu_i(t+1) = \frac{\sum_k \mathrm{P}(w_i | x_k, \lambda_t) x_k}{\sum_k \mathrm{P}(w_i | x_k, \lambda_t)}$$

E.M. for General GMMs

$p_i(t)$ is shorthand for estimate of *$P(\omega_i)$* on t' th iteration

Iterate. On the *t*' th iteration let our estimates be

$$\lambda_t = \{ \mu_1(t), \mu_2(t) \ldots \mu_c(t), \Sigma_1(t), \Sigma_2(t) \ldots \Sigma_c(t), p_1(t), p_2(t) \ldots p_c(t) \}$$

E-step: Compute "expected" clusters of all datapoints

Just evaluate a Gaussian at x_k

$$P(w_i \mid x_k, \lambda_t) = \frac{p(x_k \mid w_i, \lambda_t) P(w_i \mid \lambda_t)}{p(x_k \mid \lambda_t)} = \frac{p(x_k \mid w_i, \mu_i(t), \Sigma_i(t)) p_i(t)}{\sum_{j=1}^{c} p(x_k \mid w_j, \mu_j(t), \Sigma_j(t)) p_j(t)}$$

M-step: Estimate **μ, Σ** given our data's class membership distributions

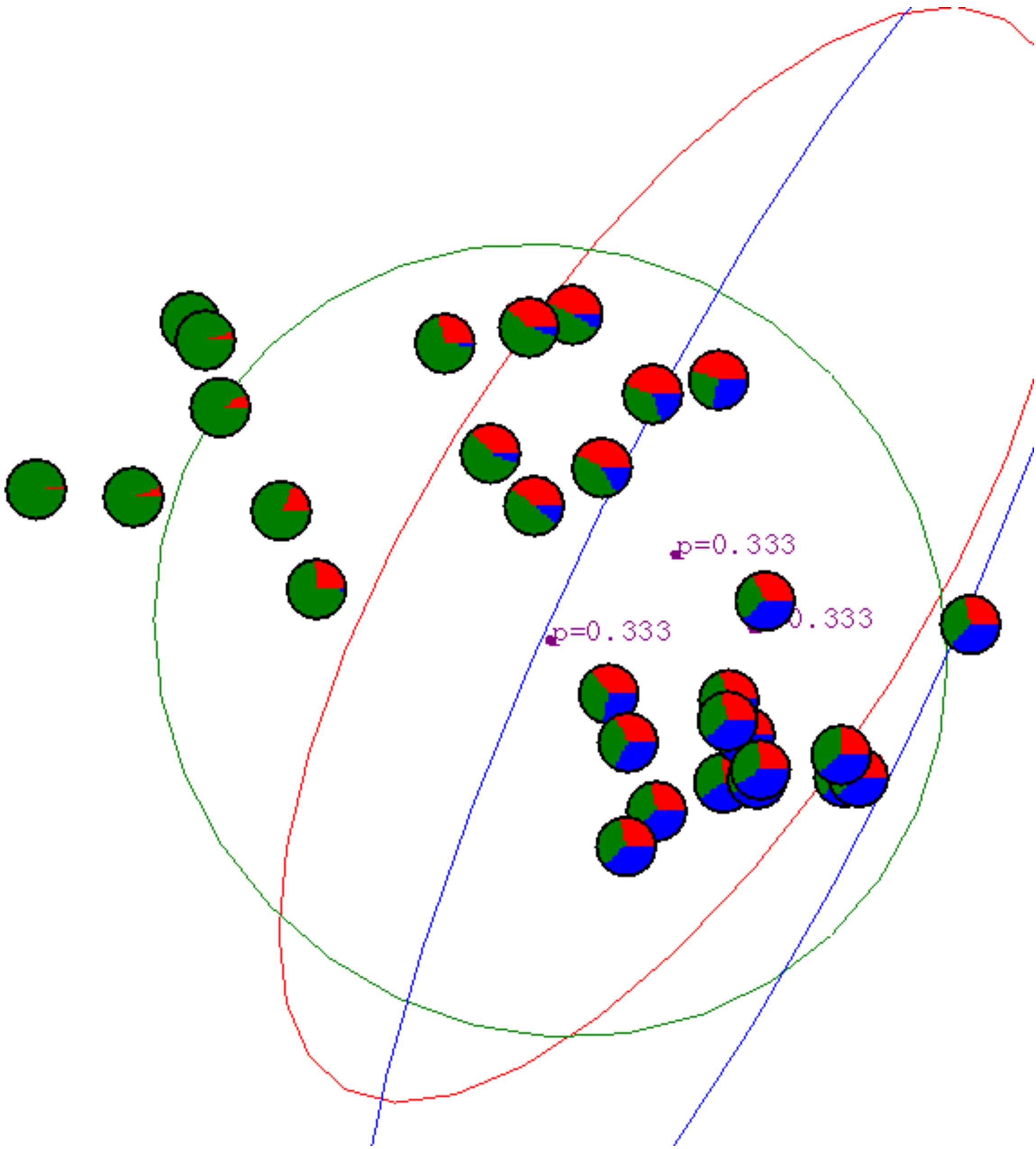
$$\mu_i(t+1) = \frac{\sum_k P(w_i \mid x_k, \lambda_t) x_k}{\sum_k P(w_i \mid x_k, \lambda_t)} \qquad \Sigma_i(t+1) = \frac{\sum_k P(w_i \mid x_k, \lambda_t) [x_k - \mu_i(t+1)][x_k - \mu_i(t+1)]^T}{\sum_k P(w_i \mid x_k, \lambda_t)}$$

$$p_i(t+1) = \frac{\sum_k P(w_i \mid x_k, \lambda_t)}{R}$$

R = #records

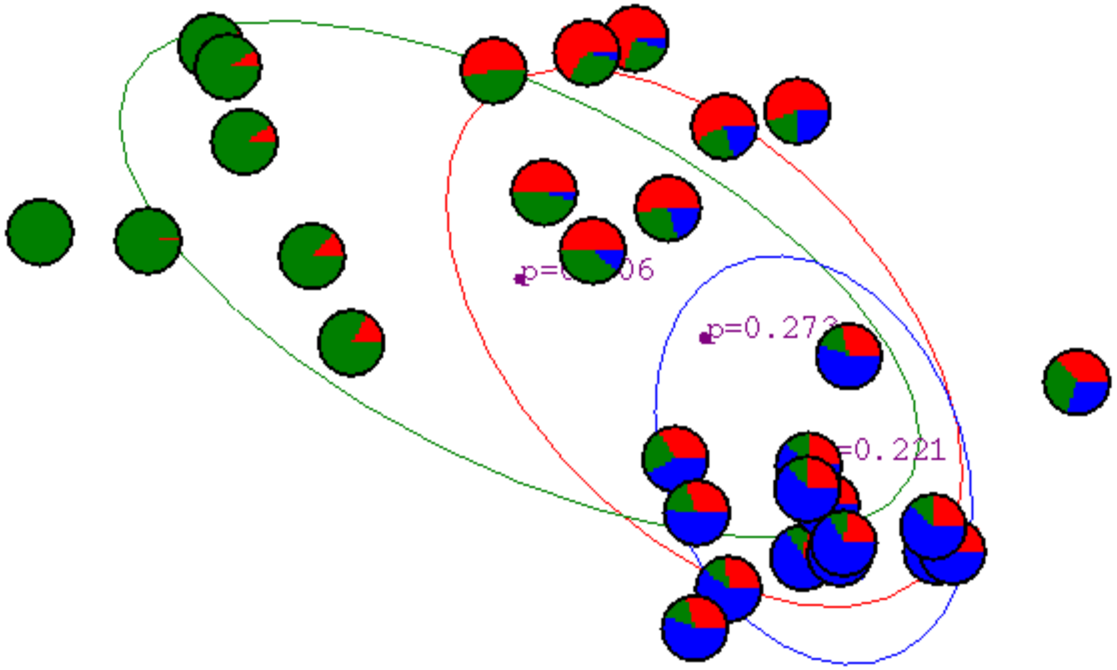
(End optional section)

Gaussian Mixture Example: Start

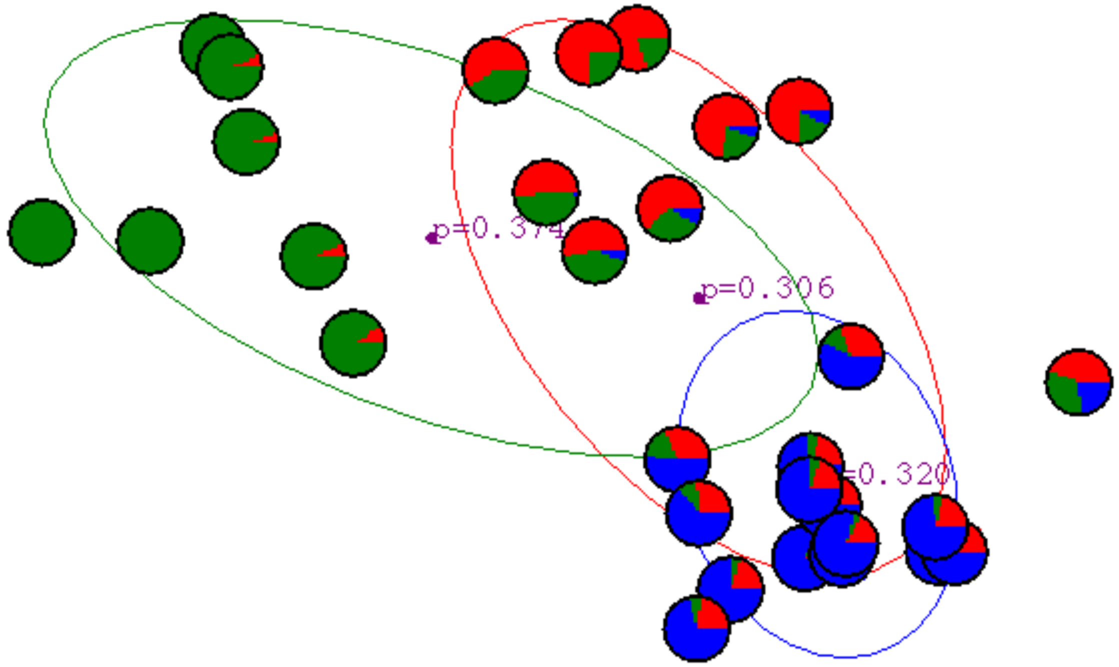


Advance apologies: in Black and White this example will be incomprehensible

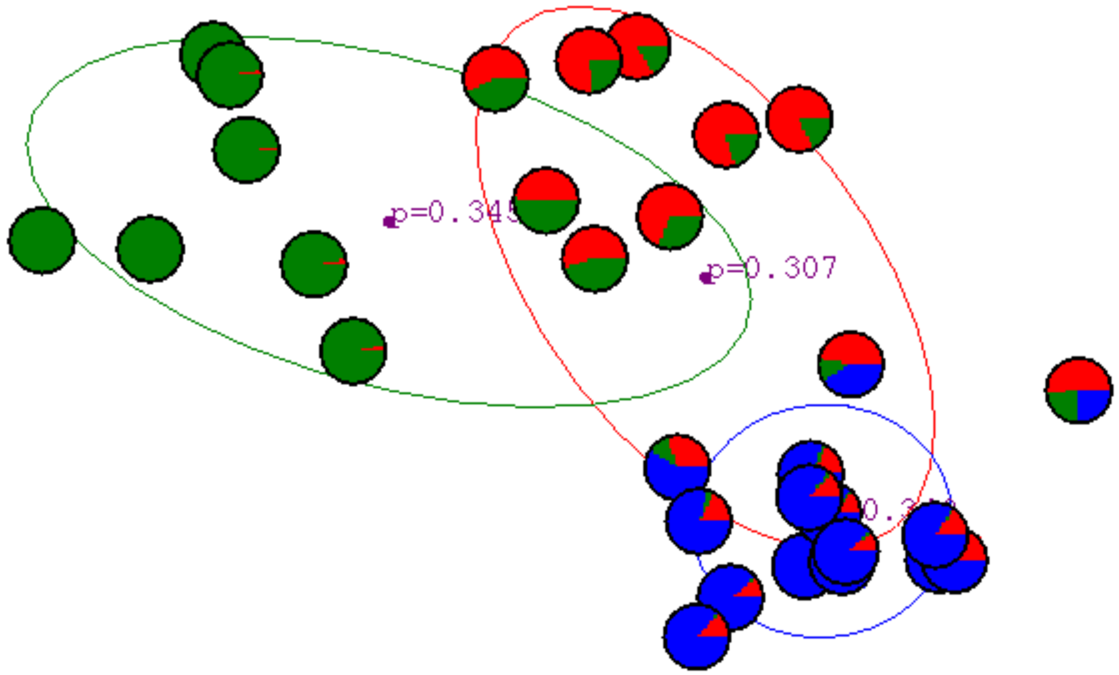
After first iteration



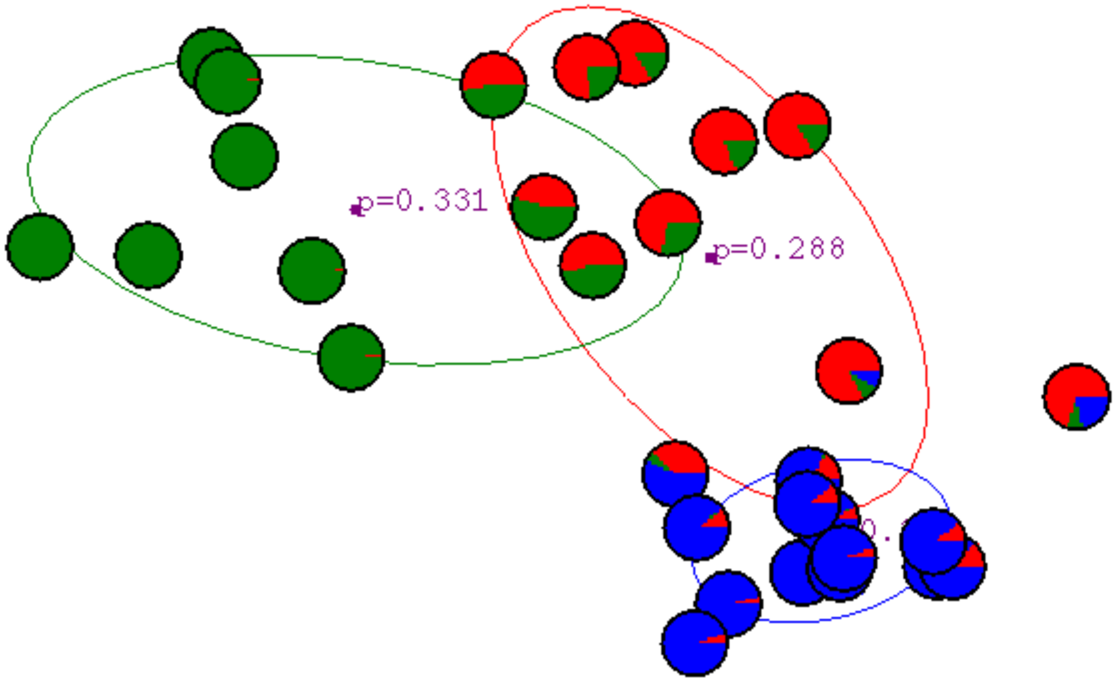
After 2nd iteration



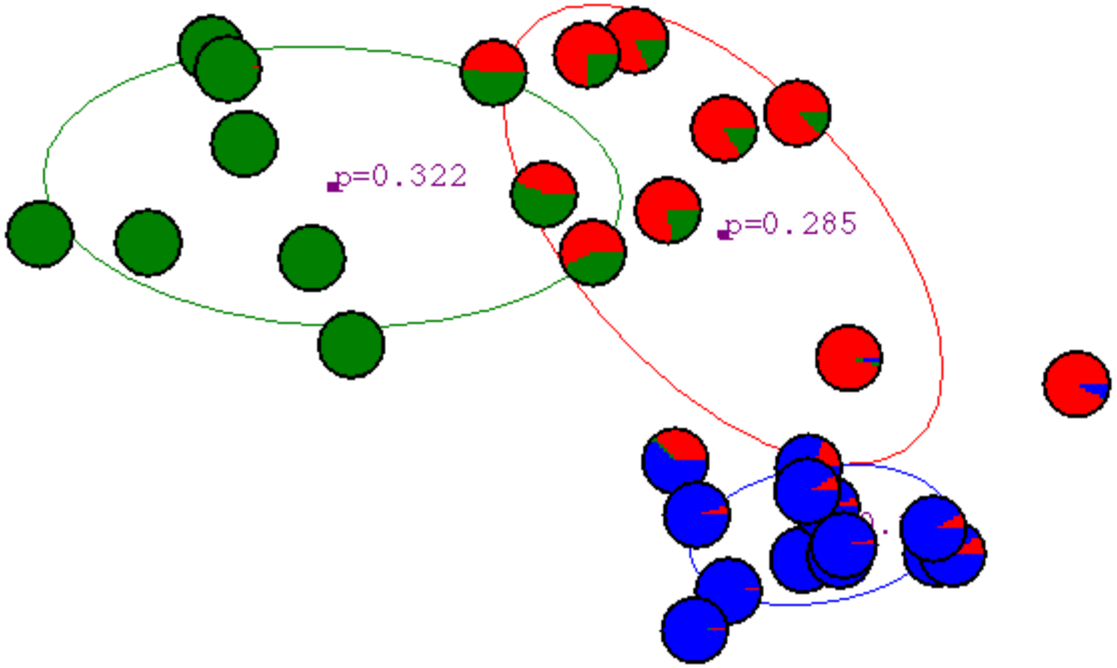
After 3rd iteration



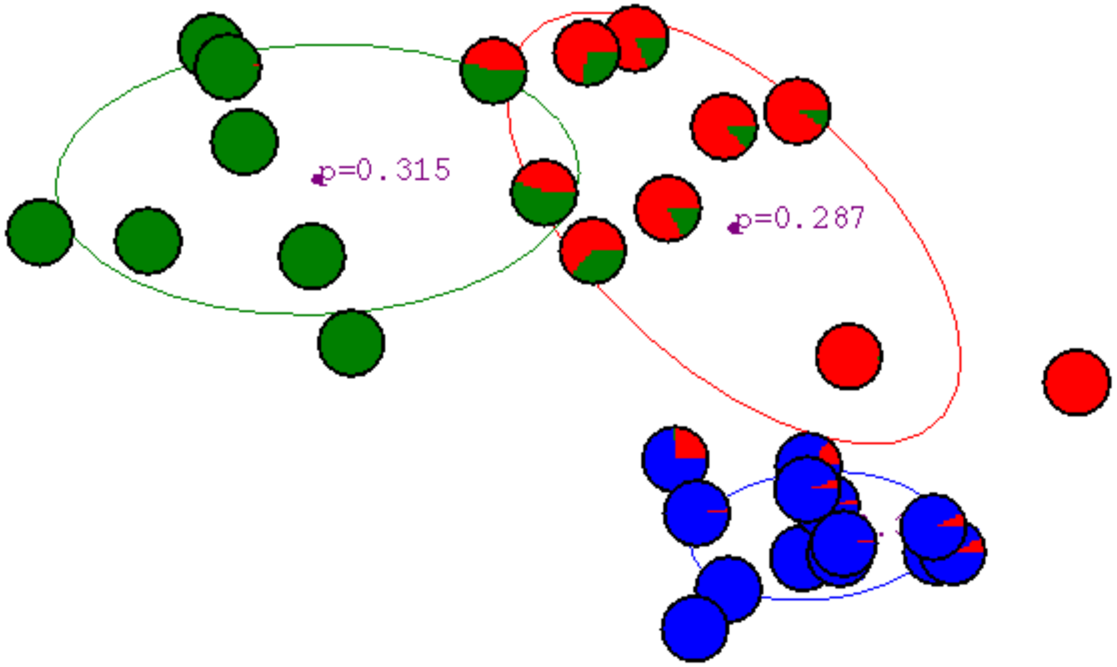
After 4th iteration



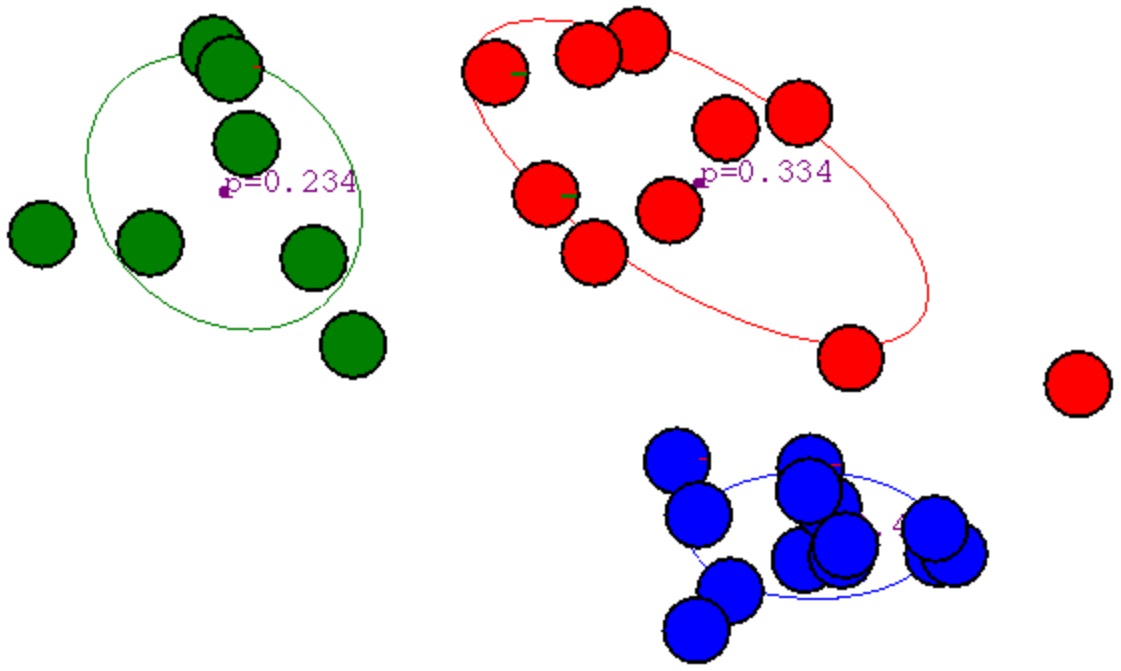
After 5th iteration



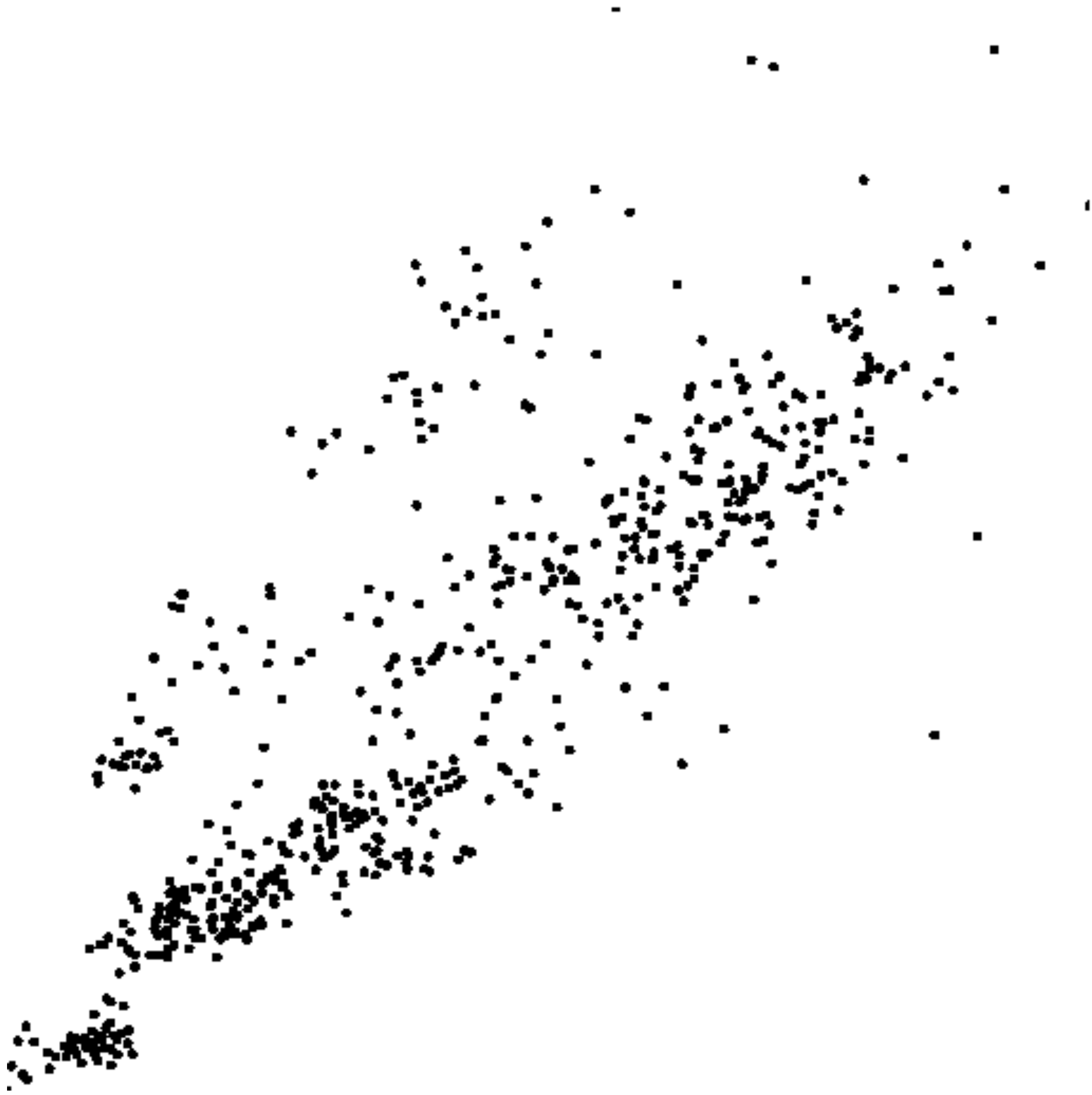
After 6th iteration



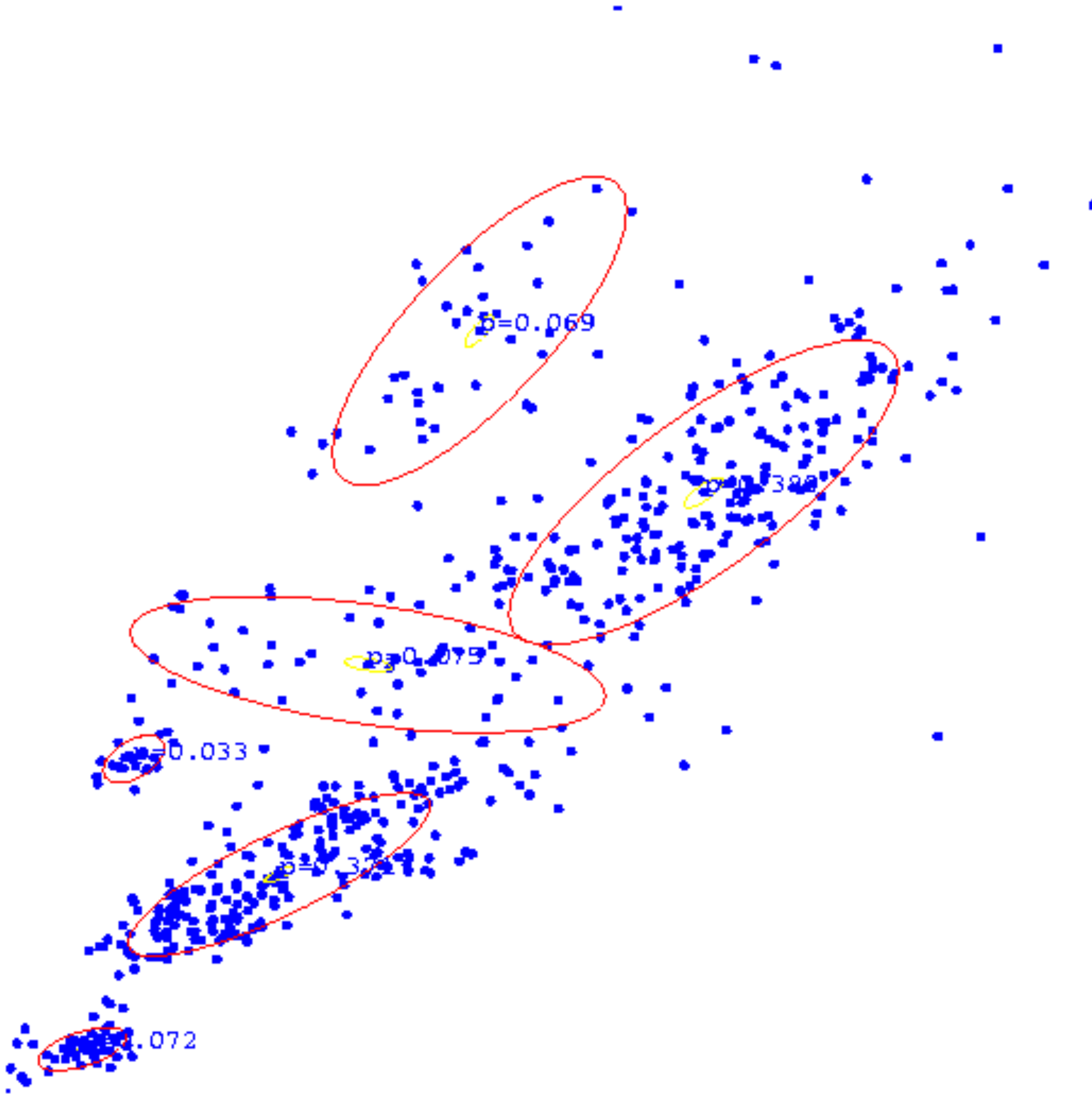
After 20th iteration



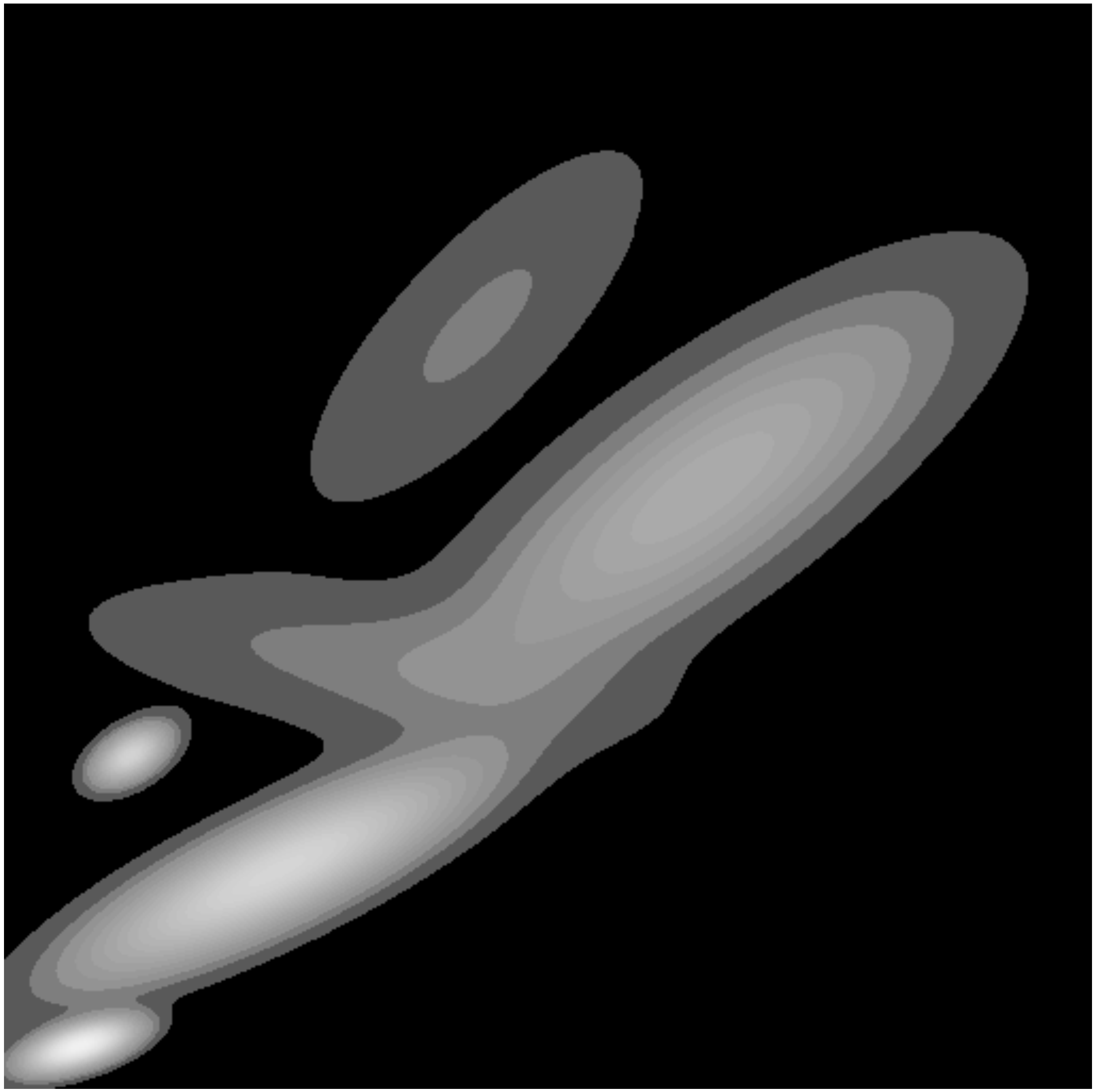
Some Bio Assay data



GMM clustering of the assay data



Resulting Density Estimator



Principal Components Analysis

Based on slides by Barnabás Póczos, UAlberta

How Can We Visualize High Dimensional Data?

- E.g., 53 blood and urine tests for 65 patients

Instances

	H-WBC	H-RBC	H-Hgb	H-Hct	H-MCV	H-MCH	H-MCHC
A1	8.0000	4.8200	14.1000	41.0000	85.0000	29.0000	34.0000
A2	7.3000	5.0200	14.7000	43.0000	86.0000	29.0000	34.0000
A3	4.3000	4.4800	14.1000	41.0000	91.0000	32.0000	35.0000
A4	7.5000	4.4700	14.9000	45.0000	101.0000	33.0000	33.0000
A5	7.3000	5.5200	15.4000	46.0000	84.0000	28.0000	33.0000
A6	6.9000	4.8600	16.0000	47.0000	97.0000	33.0000	34.0000
A7	7.8000	4.6800	14.7000	43.0000	92.0000	31.0000	34.0000
A8	8.6000	4.8200	15.8000	42.0000	88.0000	33.0000	37.0000
A9	5.1000	4.7100	14.0000	43.0000	92.0000	30.0000	32.0000

Features

Difficult to see the correlations between the features...

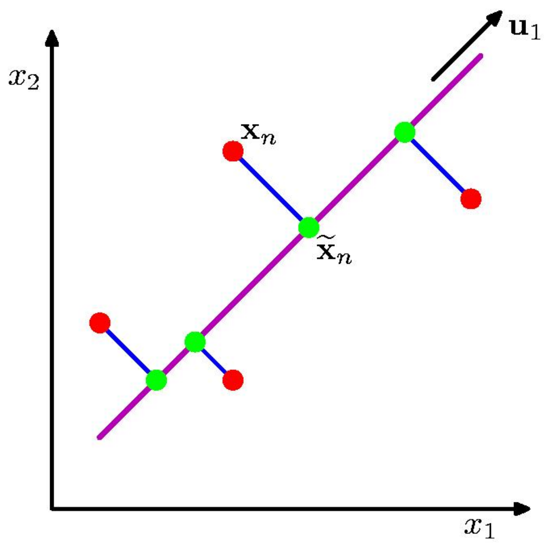
Data Visualization

- Is there a representation better than the raw features?
  - Is it really necessary to show all the 53 dimensions?
  - … what if there are strong correlations between the features?

Could we find the *smallest* subspace of the 53-D space that keeps the *most information* about the original data?

One solution: **Principal Component Analysis**

Principle Component Analysis



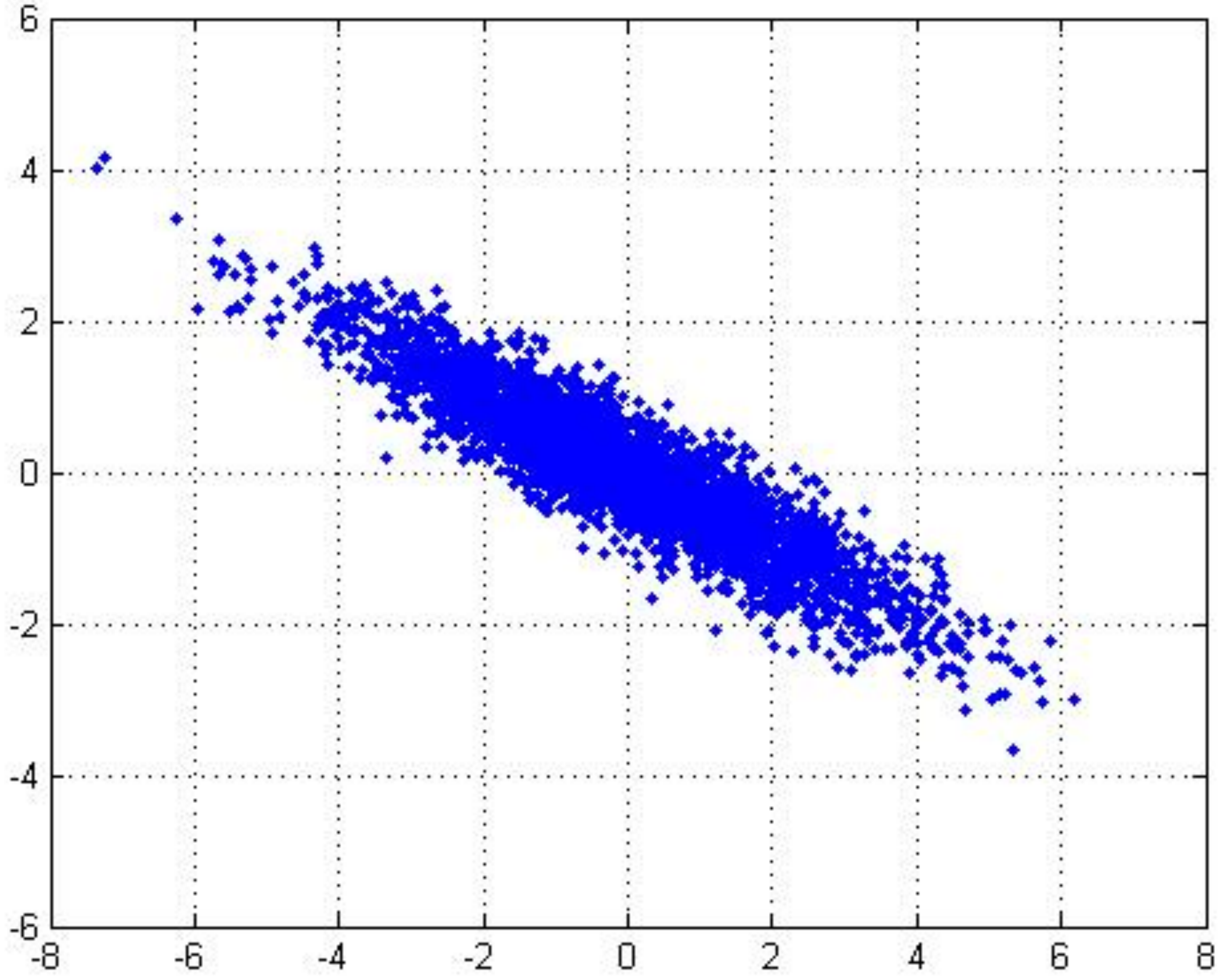
Orthogonal projection of data onto lower-dimension linear space that...

- maximizes variance of projected data (purple line)
- minimizes mean squared distance between data point and projections (sum of blue lines)

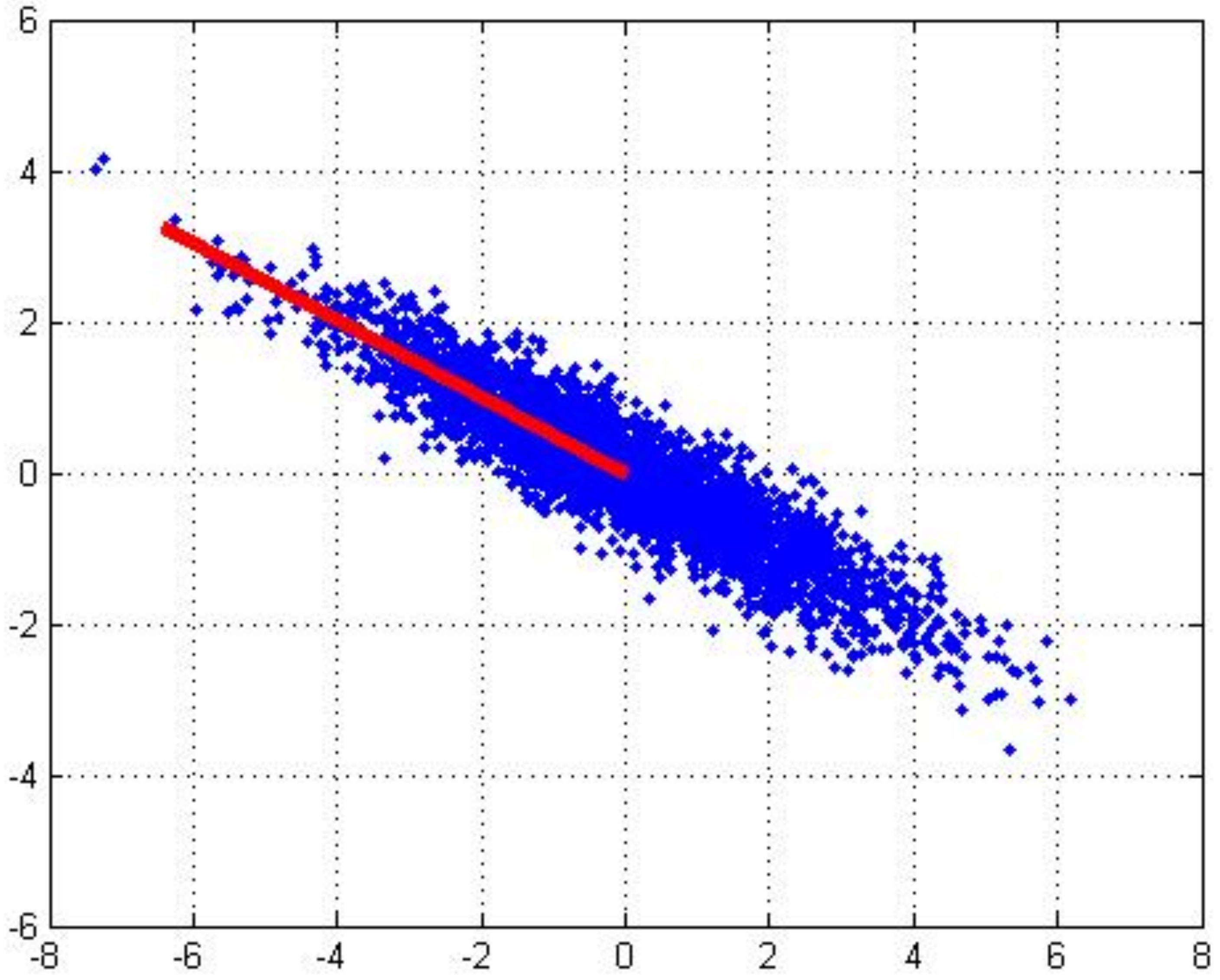
The Principal Components

- **Vectors** originating from the center of mass
- Principal component #1 points in the direction of the **largest variance**
- Each subsequent principal component…
  - is **orthogonal** to the previous ones, and
  - points in the directions of the **largest variance of the residual subspace**

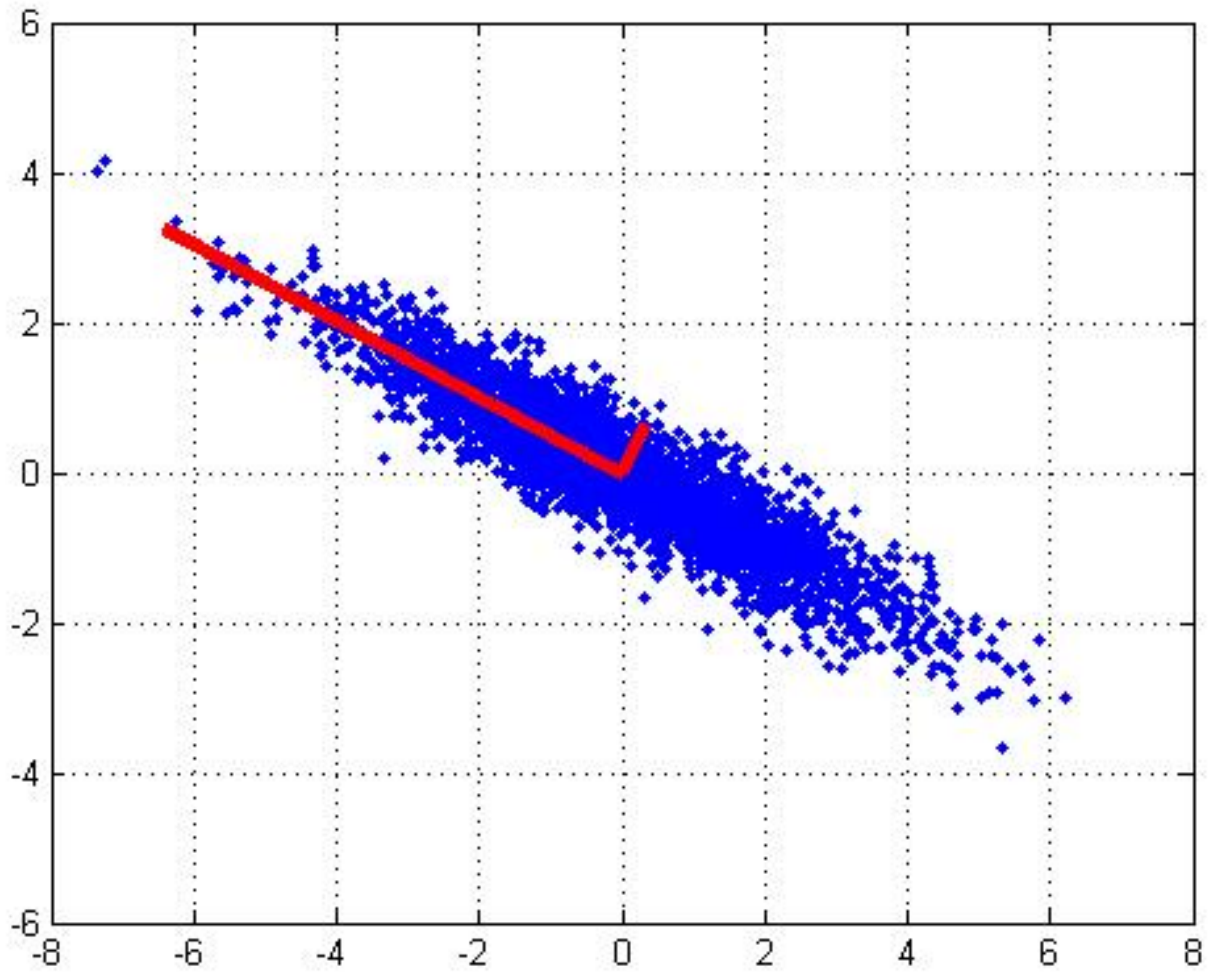
2D Gaussian Dataset



1st PCA axis

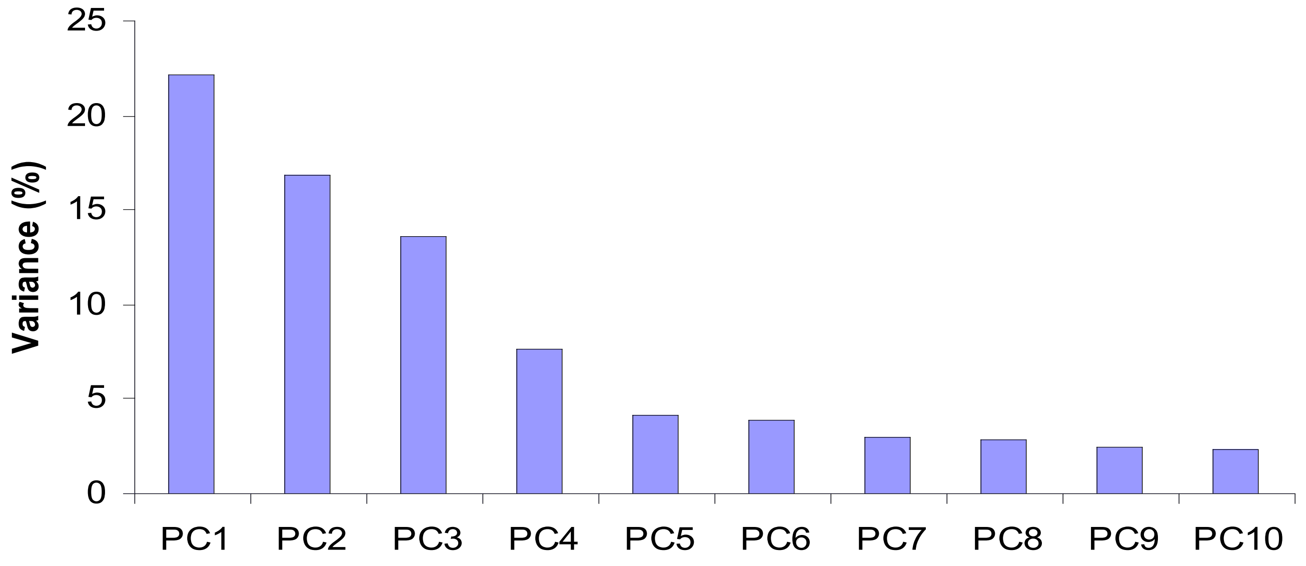


2nd PCA axis



Dimensionality Reduction

Can *ignore* the components of lesser significance



You do lose some information, but if the eigenvalues are small, you don't lose much

- choose only the first k eigenvectors, based on their eigenvalues
- final data set has only k dimensions

PCA Algorithm

- Given data $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, compute covariance matrix $\boldsymbol{\Sigma}$
  - X is the n x d data matrix
  - Compute data mean (average over all rows of X)
  - Subtract mean from each row of X (centering the data)
  - Compute covariance matrix $\boldsymbol{\Sigma} = \mathrm{X}\mathrm{X}^{\mathsf{T}}$
- **PCA** basis vectors are given by the eigenvectors of $\boldsymbol{\Sigma}$
  - $\mathrm{Q},\Lambda =$ numpy.linalg.eig(Σ)
  - $\{\mathbf{q}_i, \lambda_i\}_{i=1..n}$ are the eigenvectors/eigenvalues of $\boldsymbol{\Sigma}$ … $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$
- Larger eigenvalue $\Rightarrow$ more important eigenvectors

PCA

$$
X = \begin{array}{c} \left[\begin{matrix} 0\ 1\ 0\ 1\ 1\ 0\ 0\ 1 \ldots \\ 1\ 1\ 0\ 1\ 1\ 1\ 0\ 0 \ldots \\ 0\ 0\ 1\ 1\ 1\ 0\ 0\ 0 \ldots \\ \vdots \\ 1\ 0\ 1\ 0\ 1\ 0\ 0\ 0 \ldots \end{matrix}\right] \end{array}
\begin{array}{l} \\ \\ \mathbf{x}_3 \\ \\ \\ \end{array}
$$

Columns are ordered by importance!

$$
Q = \left[\begin{matrix} 0.34 & 0.23 & -0.30 & -0.23 & \ldots \\ 0.04 & 0.13 & -0.40 & 0.21 & \ldots \\ -0.64 & 0.93 & 0.61 & 0.28 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ -0.20 & -0.83 & 0.78 & -0.93 & \ldots \end{matrix}\right]
\begin{array}{l} \\ \\ \mathbf{x}_3 \\ \\ \\ \end{array}
$$

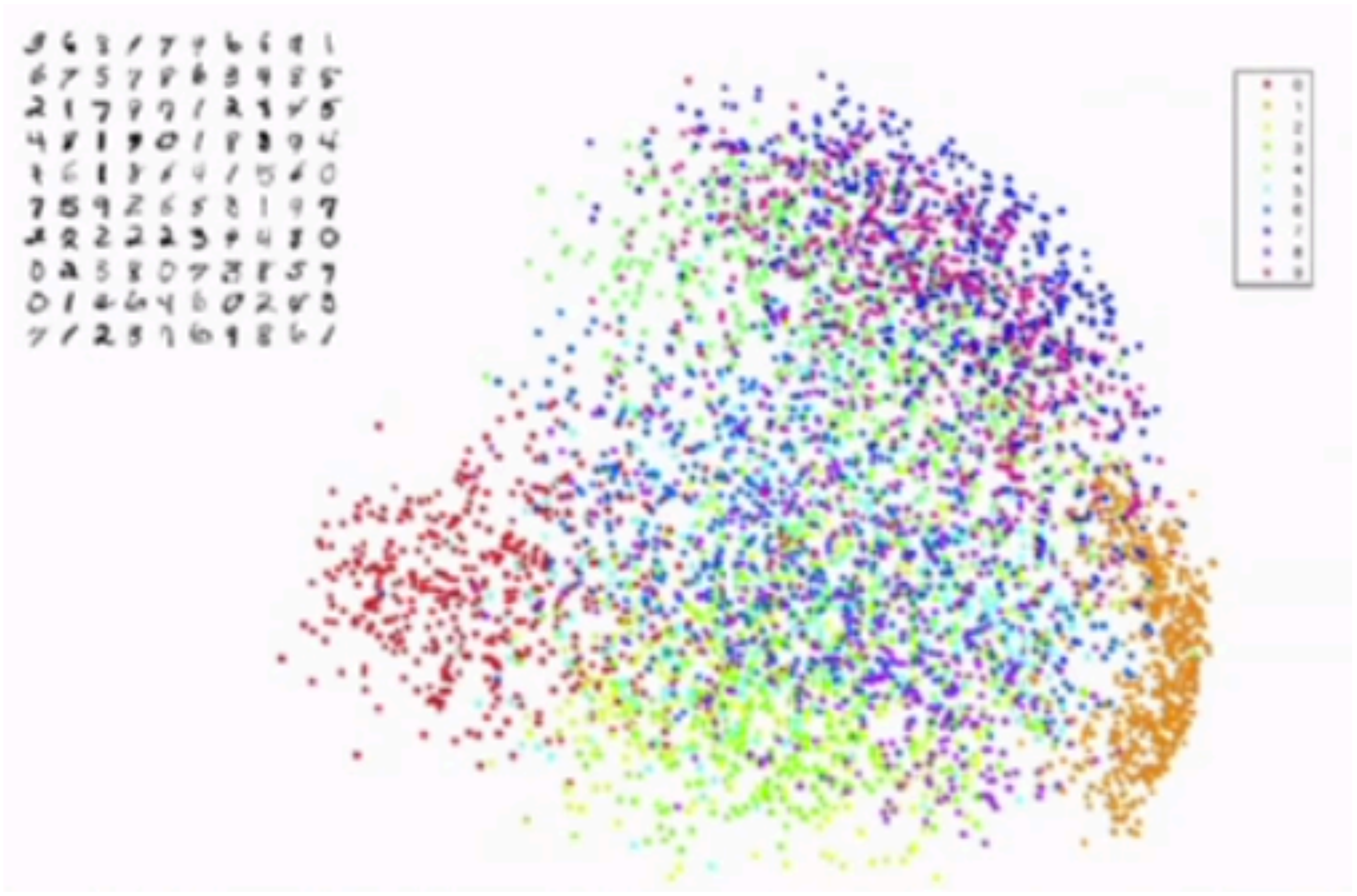
PCA

$$X = \begin{array}{c}\left[\begin{array}{c} 0\ 1\ 0\ 1\ 1\ 0\ 0\ 1 \ldots \\ 1\ 1\ 0\ 1\ 1\ 1\ 0\ 0 \ldots \\ 0\ 0\ 1\ 1\ 1\ 0\ 0\ 0 \ldots \\ \vdots \\ 1\ 0\ 1\ 0\ 1\ 0\ 0\ 0 \ldots \end{array}\right]\end{array}\begin{array}{l} \\ \\ \mathbf{x}_3 \\ \\ \\ \end{array}$$

Keep only first k columns of Q

$$Q = \left[\begin{array}{ccccc} 0.34 & 0.23 & \cancel{-0.30} & \cancel{-0.23} & \cancel{\ldots} \\ 0.04 & 0.13 & \cancel{-0.40} & \cancel{0.21} & \cancel{\ldots} \\ -0.64 & 0.93 & \cancel{0.61} & \cancel{0.28} & \cancel{\ldots} \\ \vdots & \vdots & \cancel{\vdots} & \cancel{\vdots} & \cancel{\ddots} \\ -0.20 & -0.83 & \cancel{0.78} & \cancel{-0.93} & \cancel{\ldots} \end{array}\right]\begin{array}{l} \\ \\ \mathbf{x}_3 \\ \\ \\ \end{array}$$

PCA Visualization of MNIST Digits



Challenge: Facial Recognition

- Want to identify specific person, based on facial image
- Robust to glasses, lighting,…

  ⇒ Can't just use the given 256 x 256 pixels

PCA applications -Eigenfaces

- Eigenfaces are

  the eigenvectors of

  the covariance matrix of

  the probability distribution of

  the vector space of

  human faces
- Eigenfaces are the ‘standardized face ingredients’ derived from the statistical analysis of many pictures of human faces
- A human face may be considered to be a combination of these standard faces

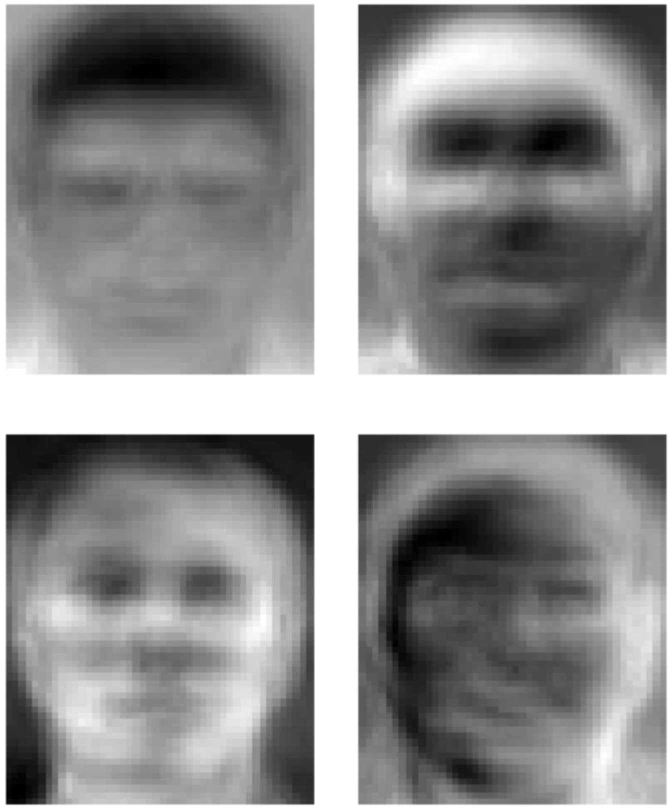
PCA applications -Eigenfaces

To generate a **set of eigenfaces:**

1. Large set of digitized images of human faces is taken under the same lighting conditions.
2. The images are normalized to line up the eyes and mouths.
3. The eigenvectors of the covariance matrix of the statistical distribution of face image vectors are then extracted.
4. These eigenvectors are called eigenfaces.

PCA applications -Eigenfaces

- the principal eigenface looks like a bland androgynous average human face



http://en.wikipedia.org/wiki/Image:Eigenfaces.png

Eigenfaces – Face Recognition

- When properly weighted, eigenfaces can be summed together to create an approximate gray-scale rendering of a human face.
- Remarkably few eigenvector terms are needed to give a fair likeness of most people's faces
- Hence eigenfaces provide a means of applying data compression to faces for identification purposes.
- Similarly, Expert Object Recognition in Video

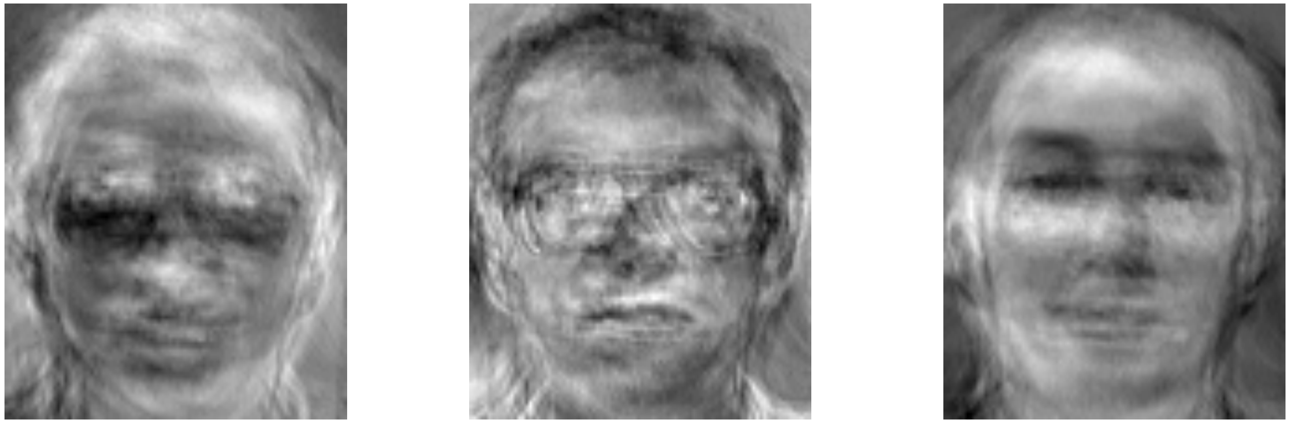
Eigenfaces

- Experiment and Results

  Data used here are from the ORL database of faces. Facial images of 16 persons each with 10 views are used. - Training set contains 16×7 images.

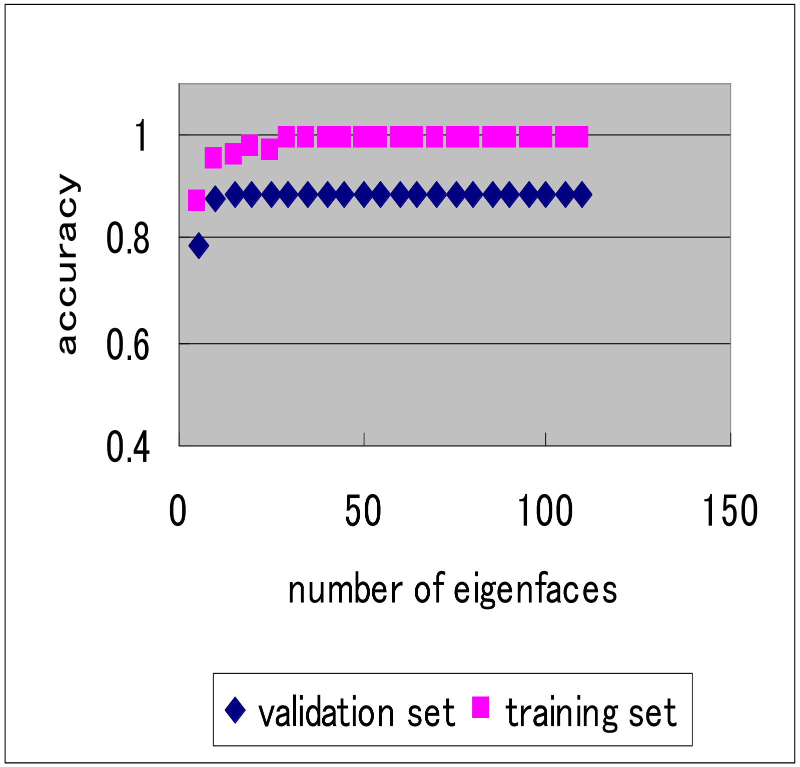
  Test set contains 16×3 images.

First three eigenfaces :



Classification Using Nearest Neighbor

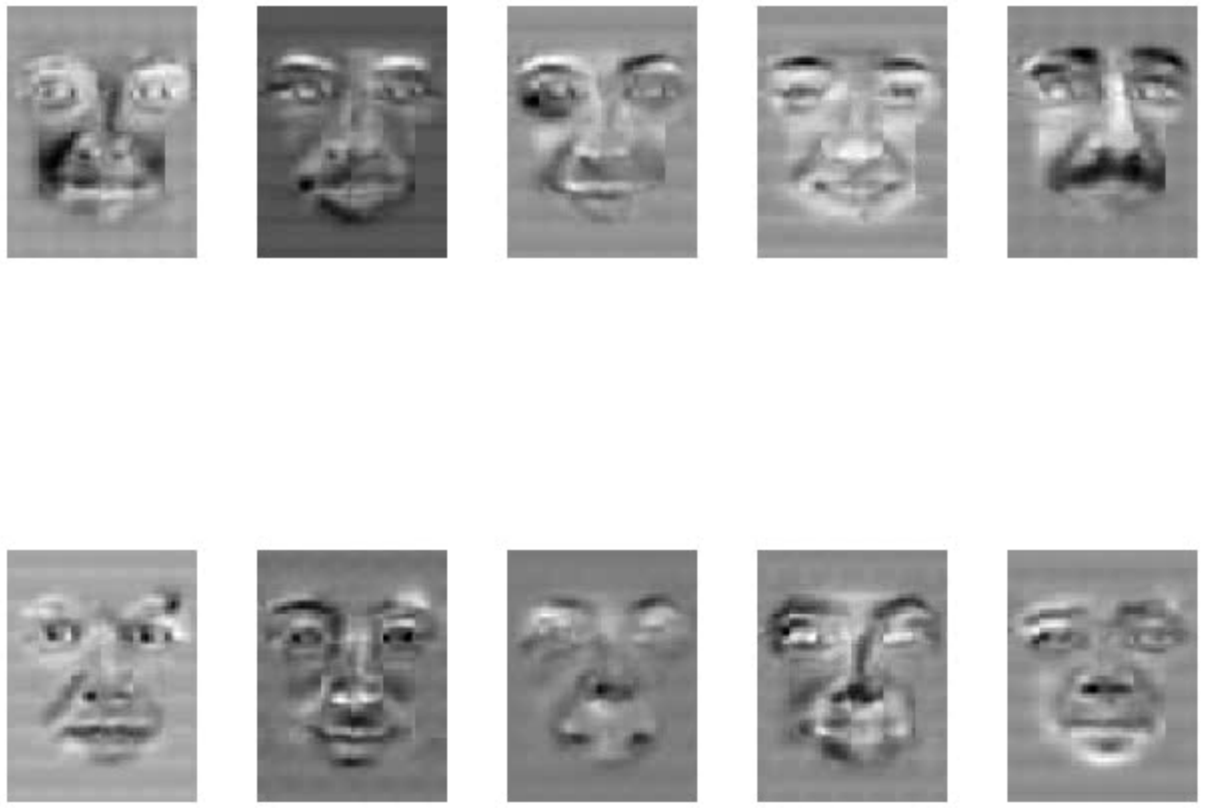
- Save average coefficients for each person. Classify new face as the person with the closest average.
- Recognition accuracy increases with number of eigenfaces till 15.
  Later eigenfaces do not help much with recognition.



Best recognition rates

Training set	99%
Test set	89%

Facial Expression Recognition: Happiness subspace



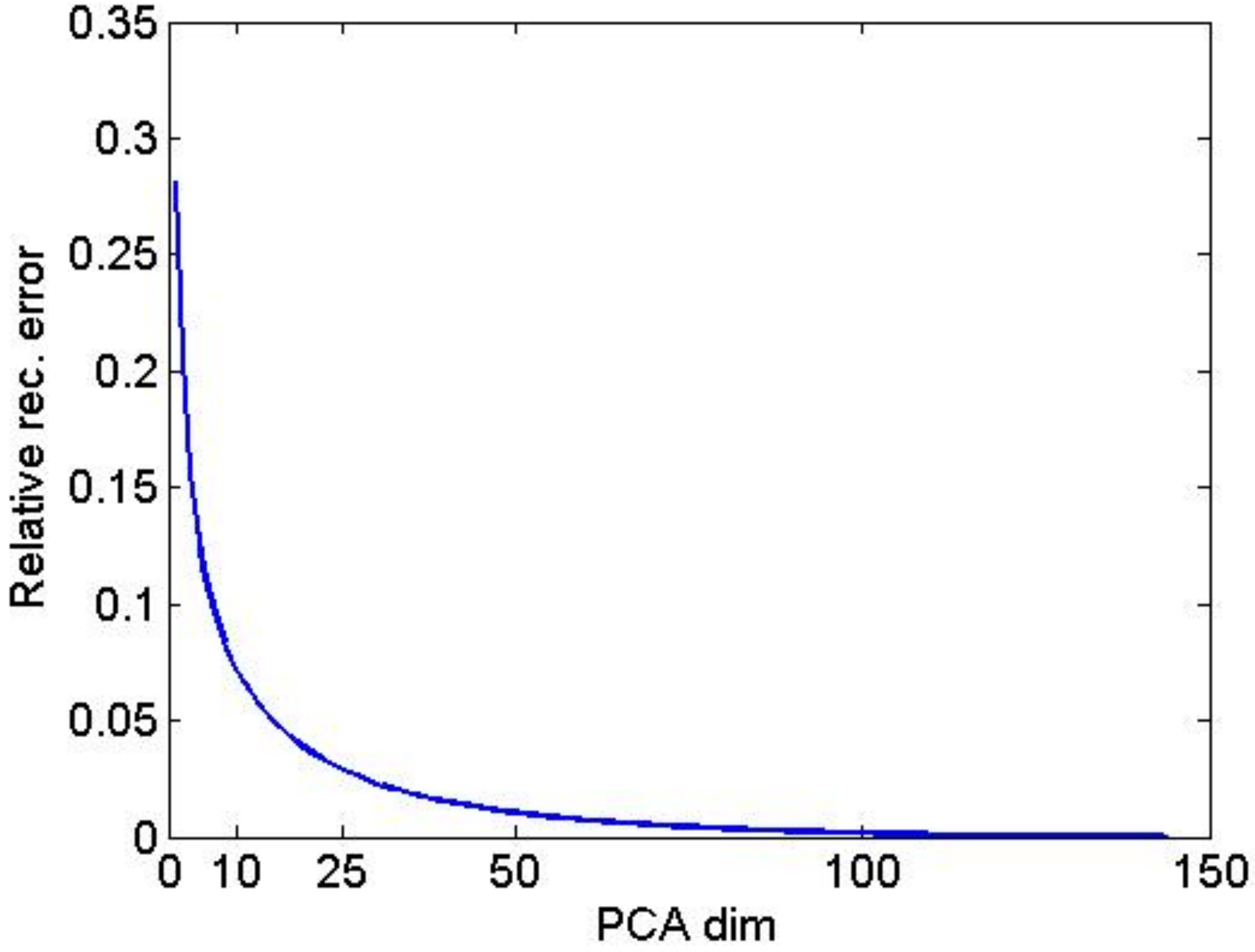
Disgust subspace

Image Compression

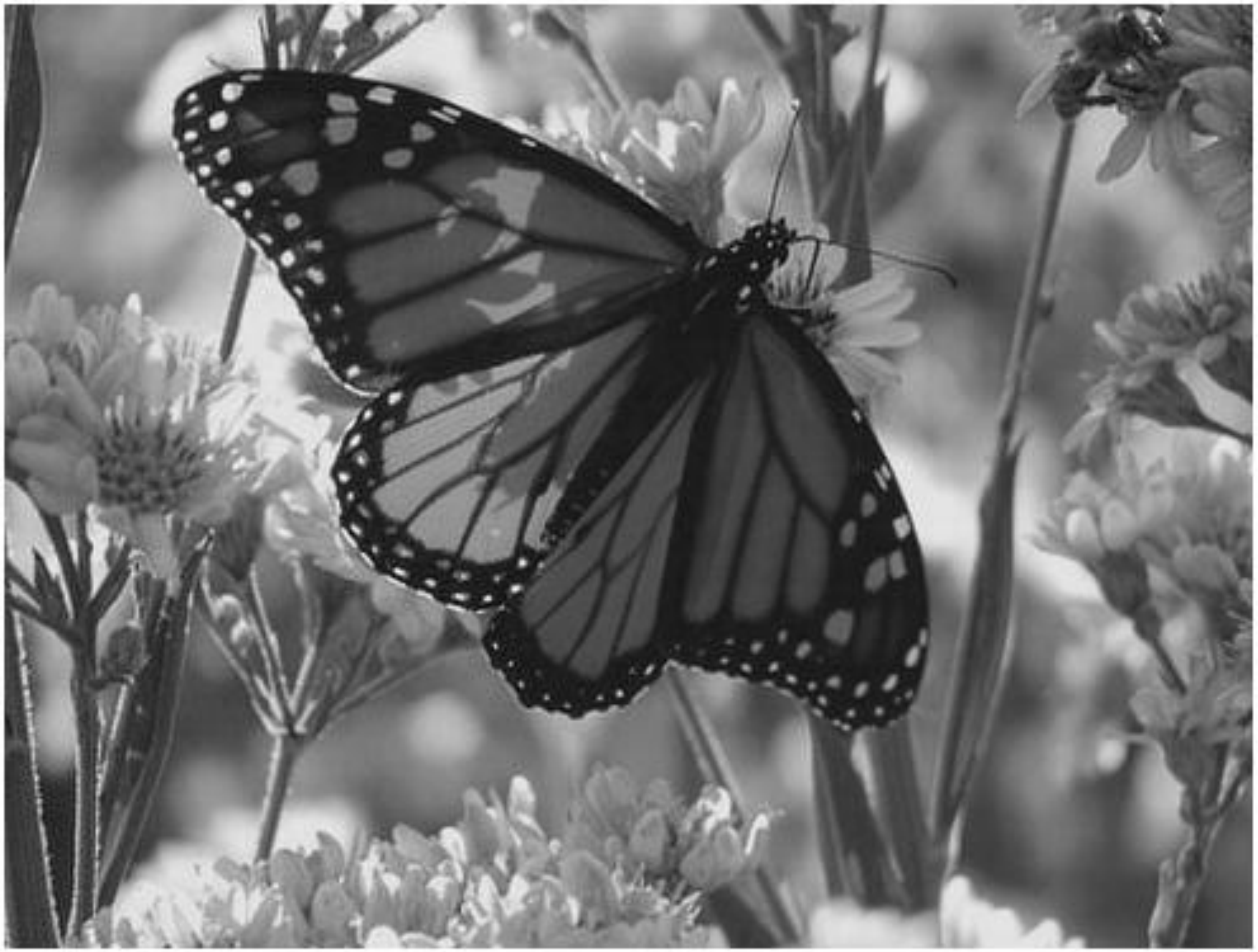
Original Image

- Divide the original 372x492 image into patches:
    - Each patch is an instance that contains 12x12 pixels on a grid
- View each as a 144-D vector

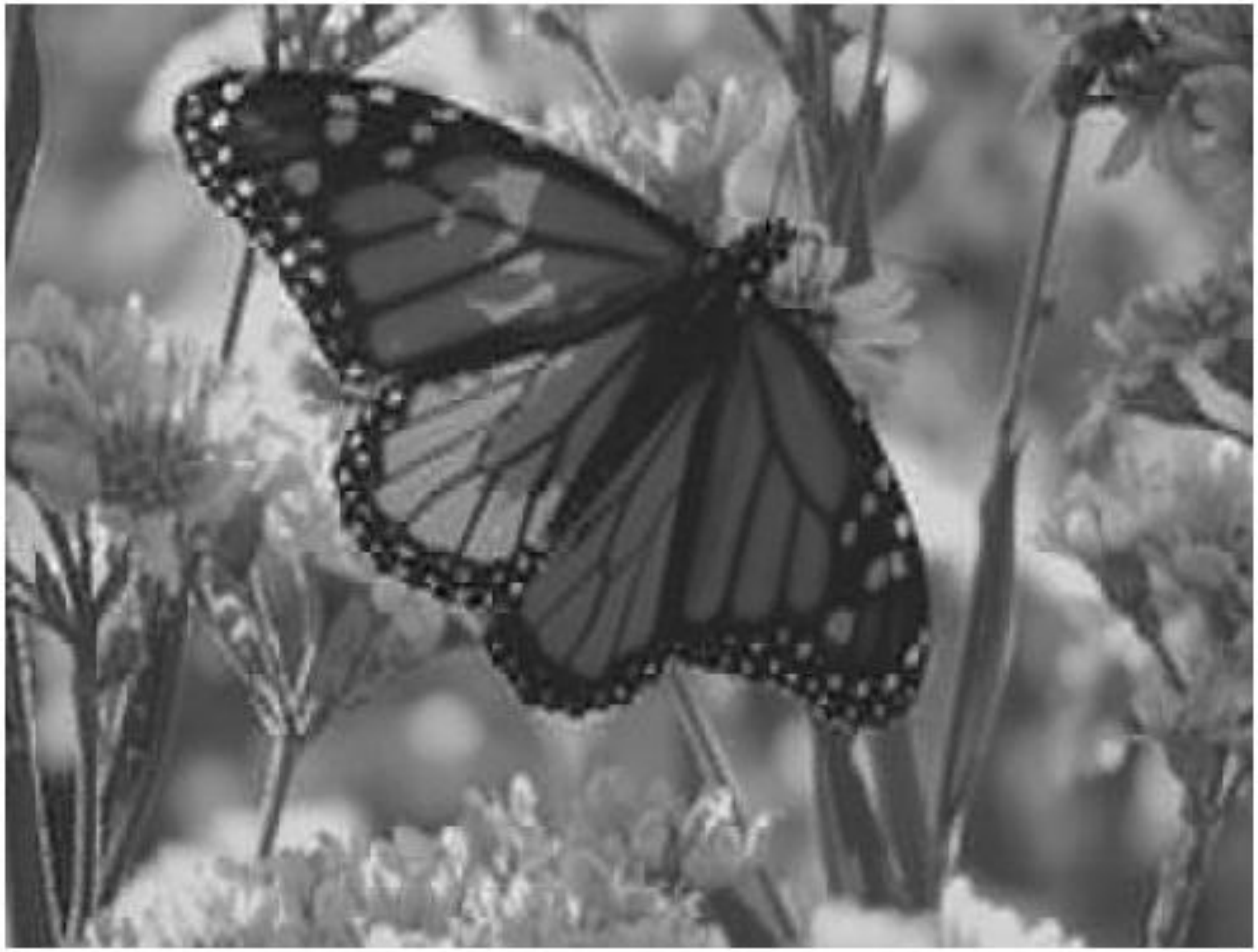
L_2 error and PCA dim



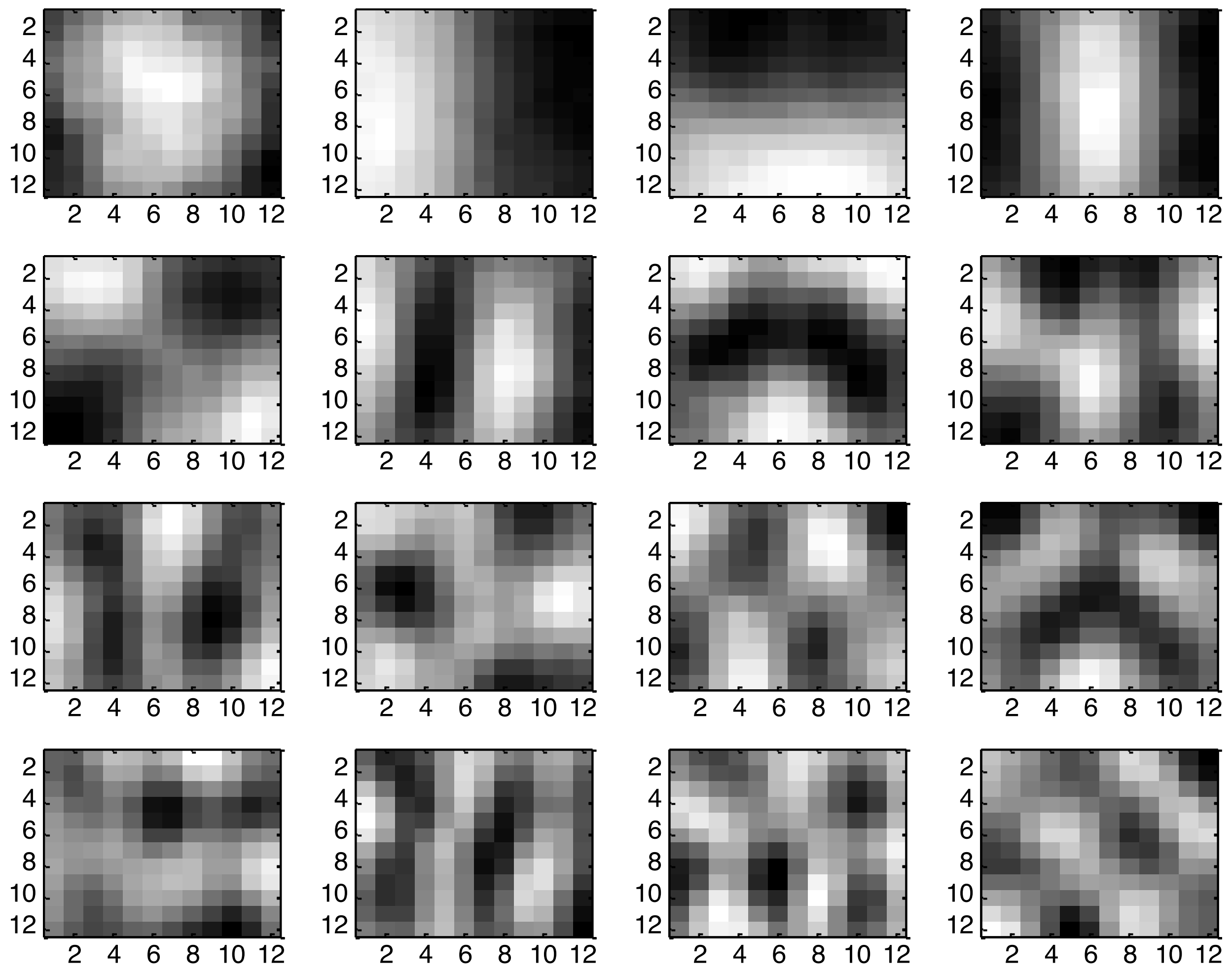
PCA compression: 144D $\Rightarrow$ 60D



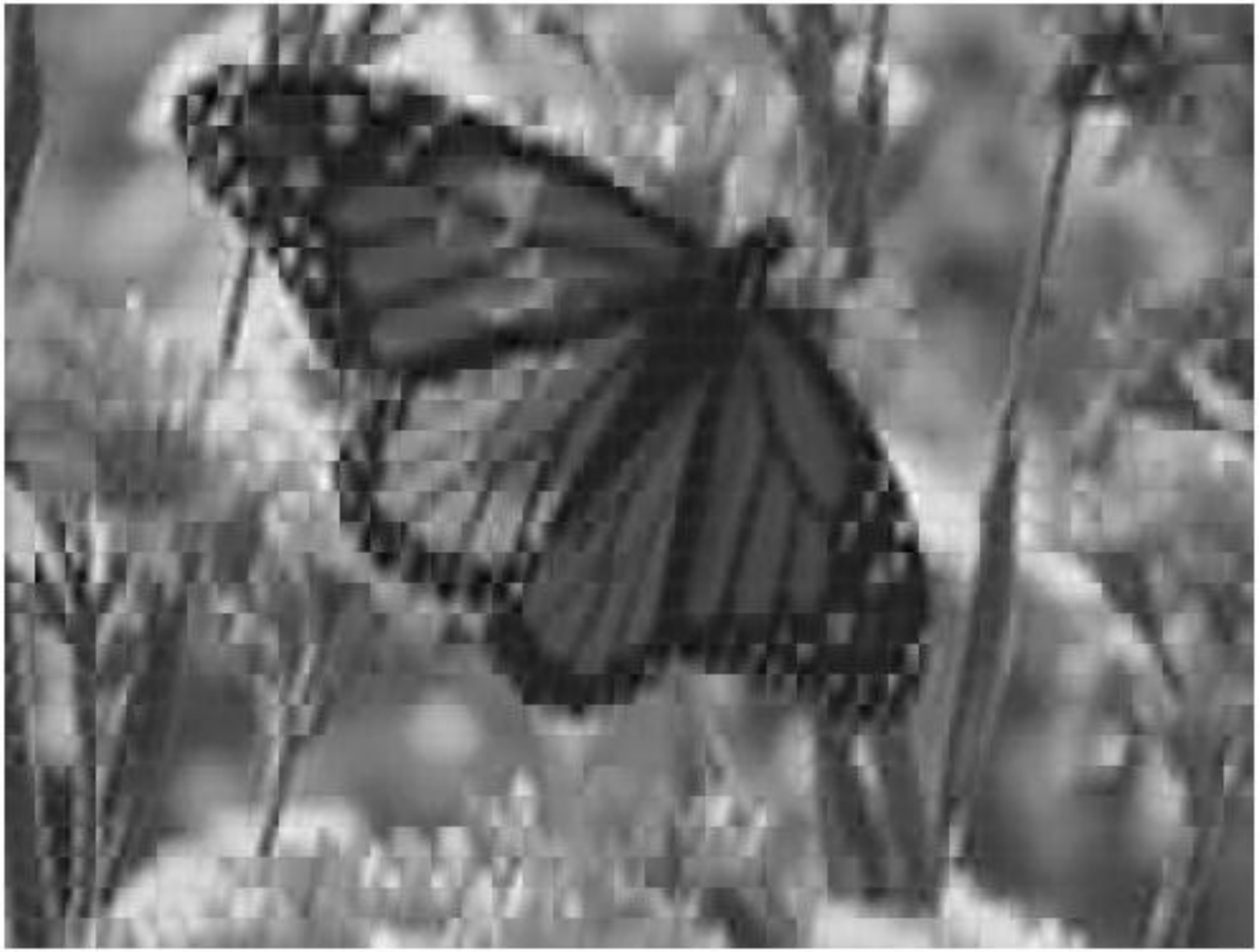
PCA compression: 144D $\Rightarrow$ 16D



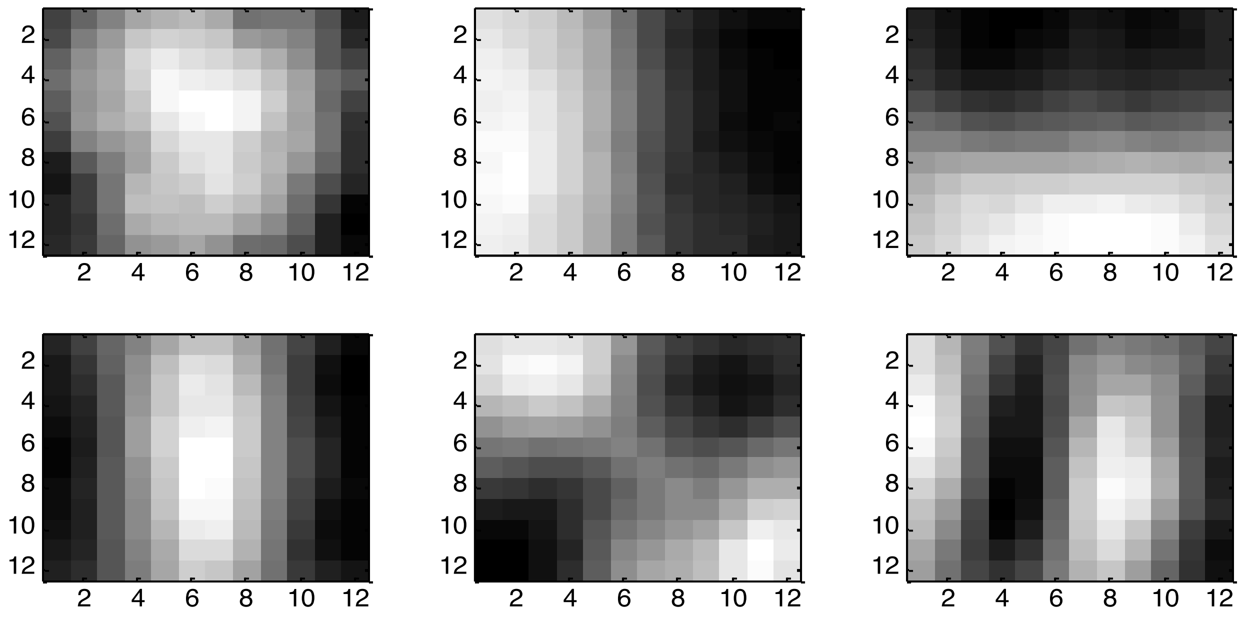
16 most important eigenvectors



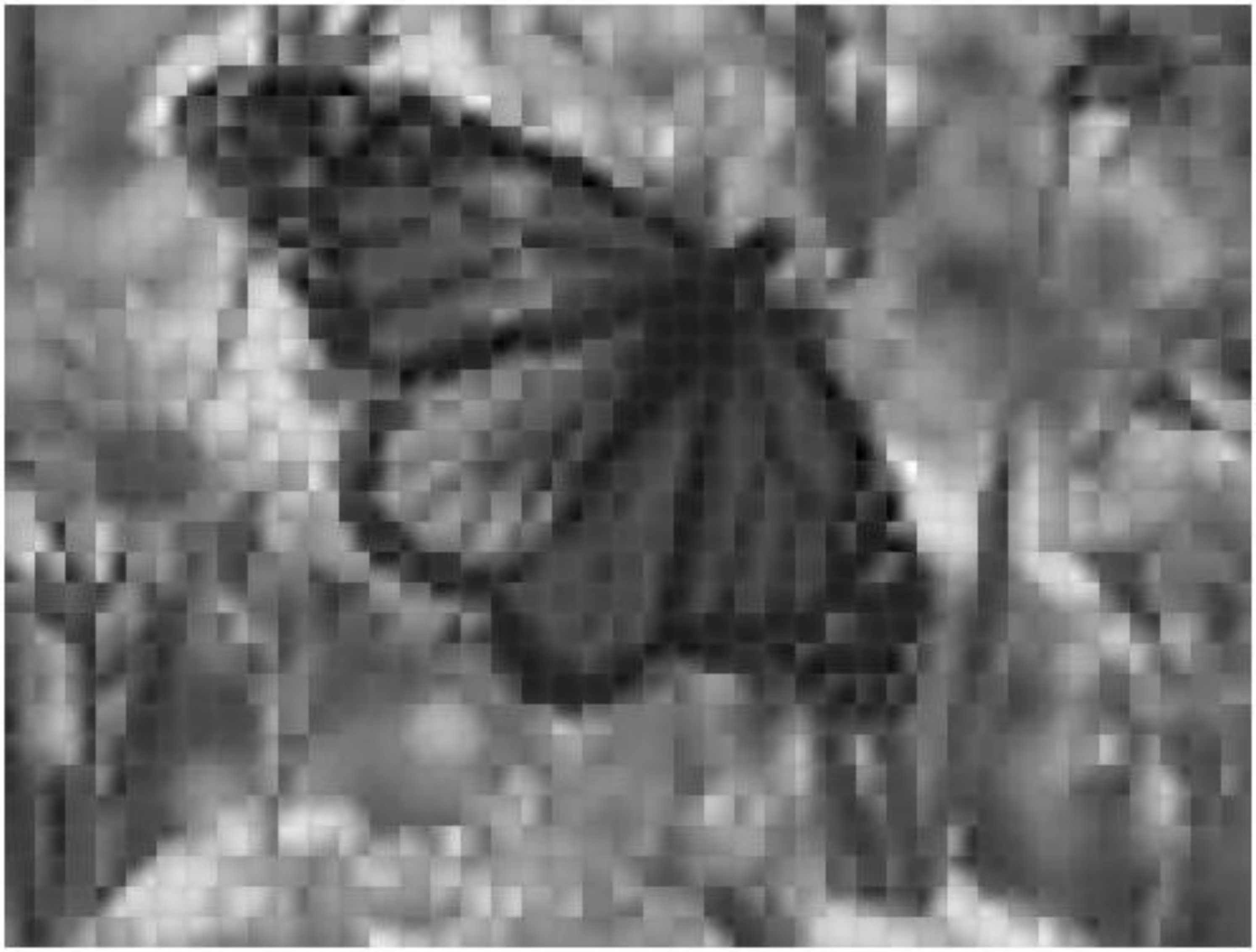
PCA compression: 144D $\Rightarrow$ 6D



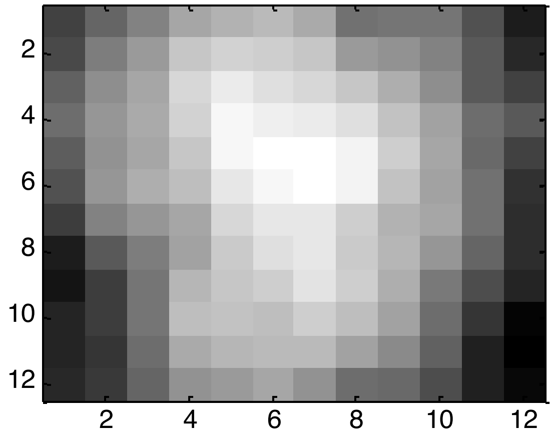
6 most important eigenvectors

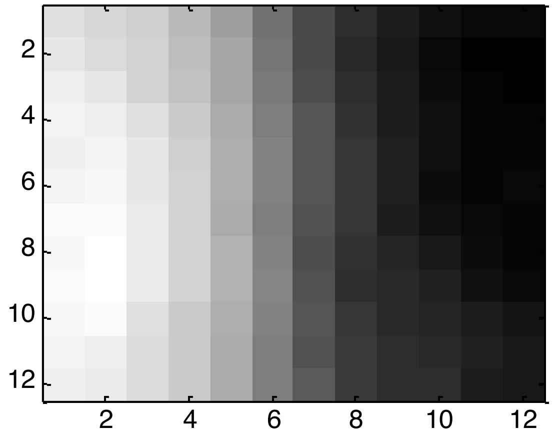


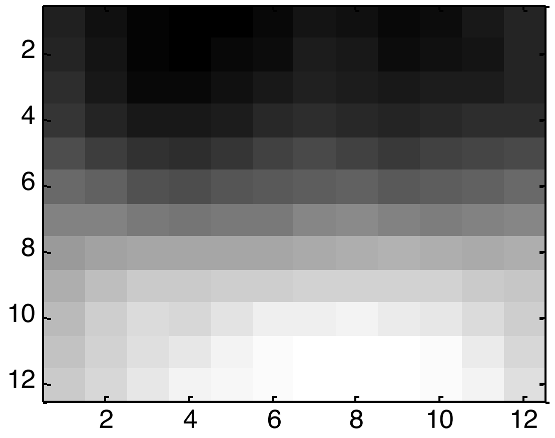
PCA compression: 144D $\Rightarrow$ 3D



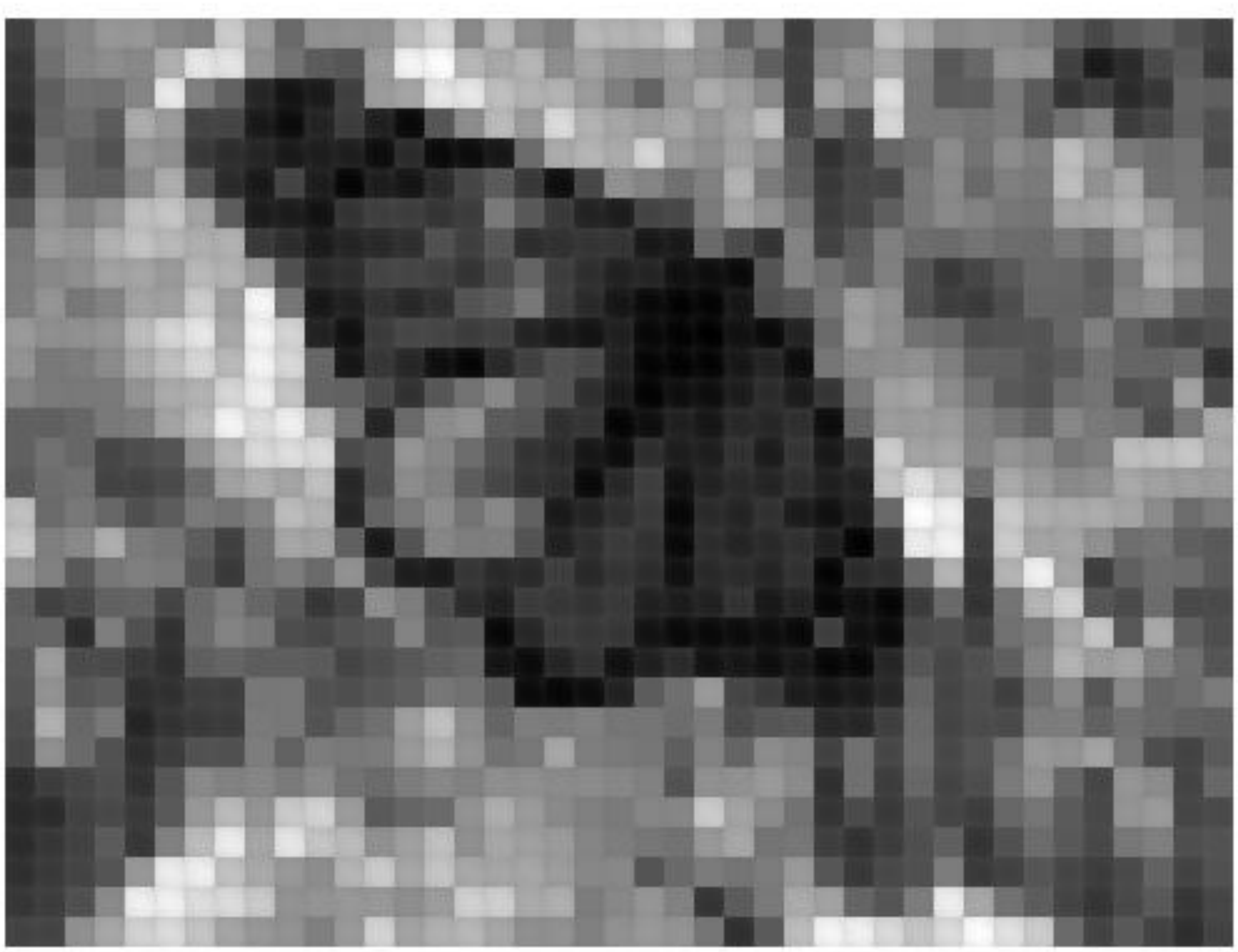
3 most important eigenvectors



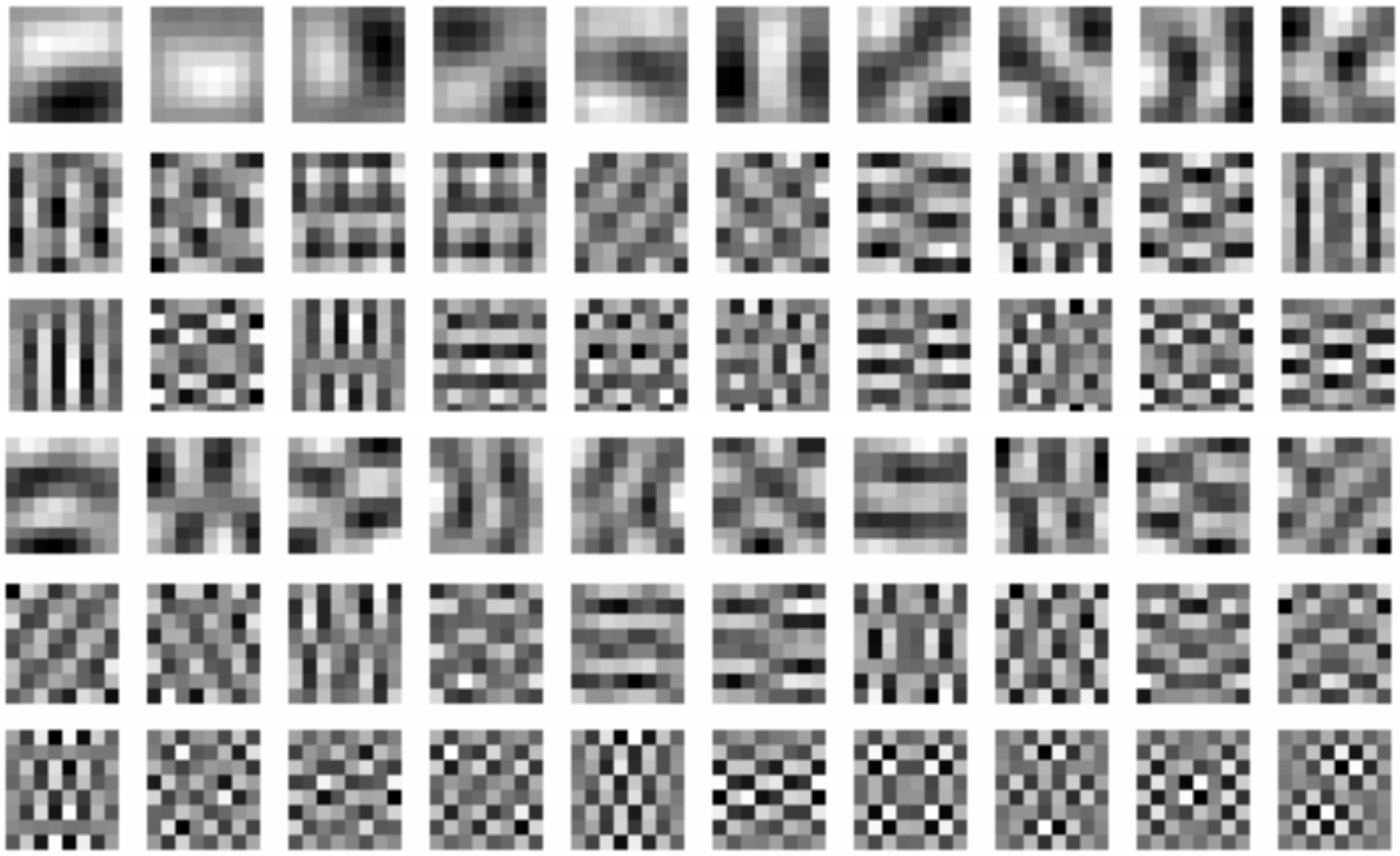




PCA compression: 144D $\Rightarrow$ 1D

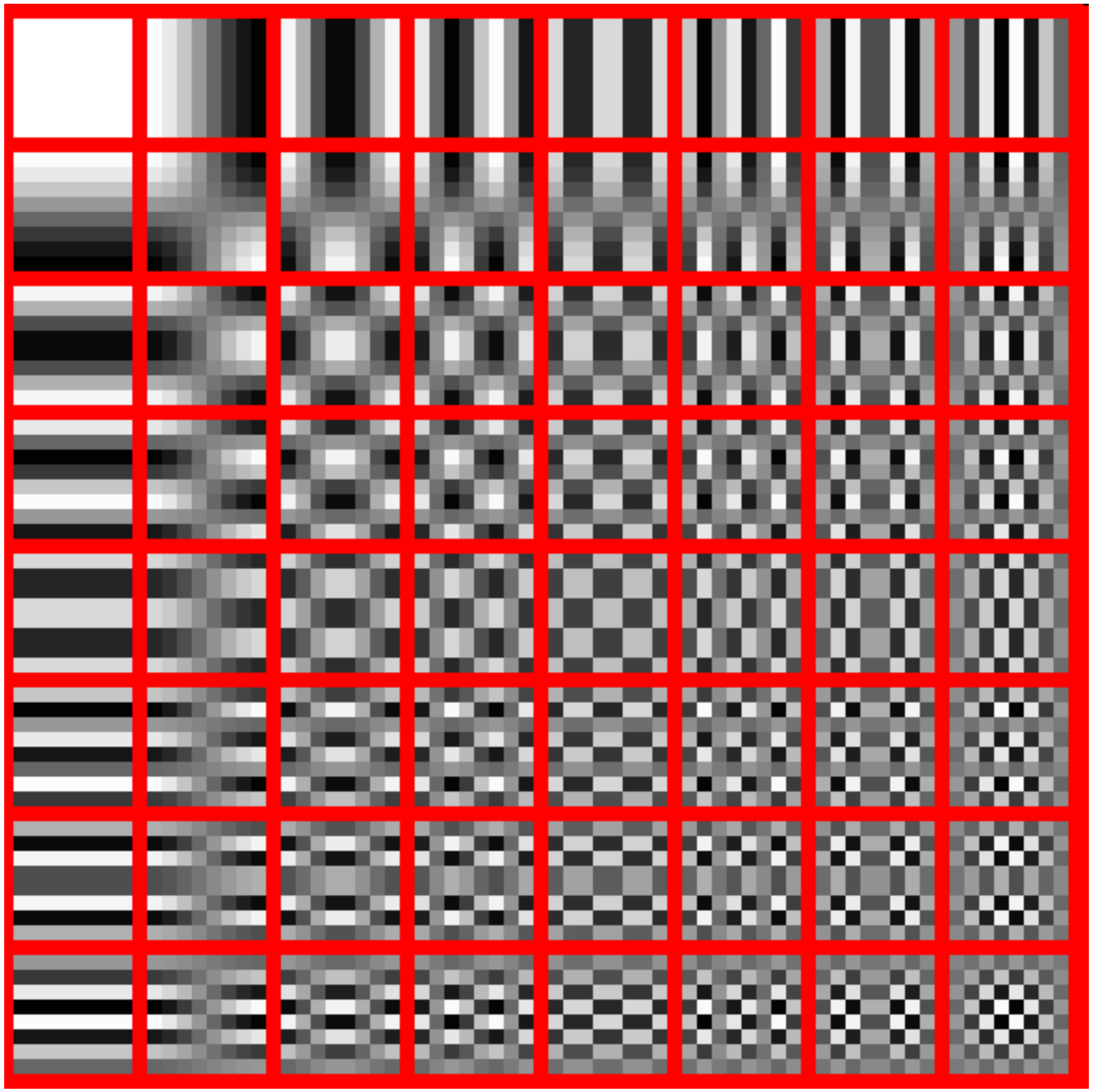


60 most important eigenvectors



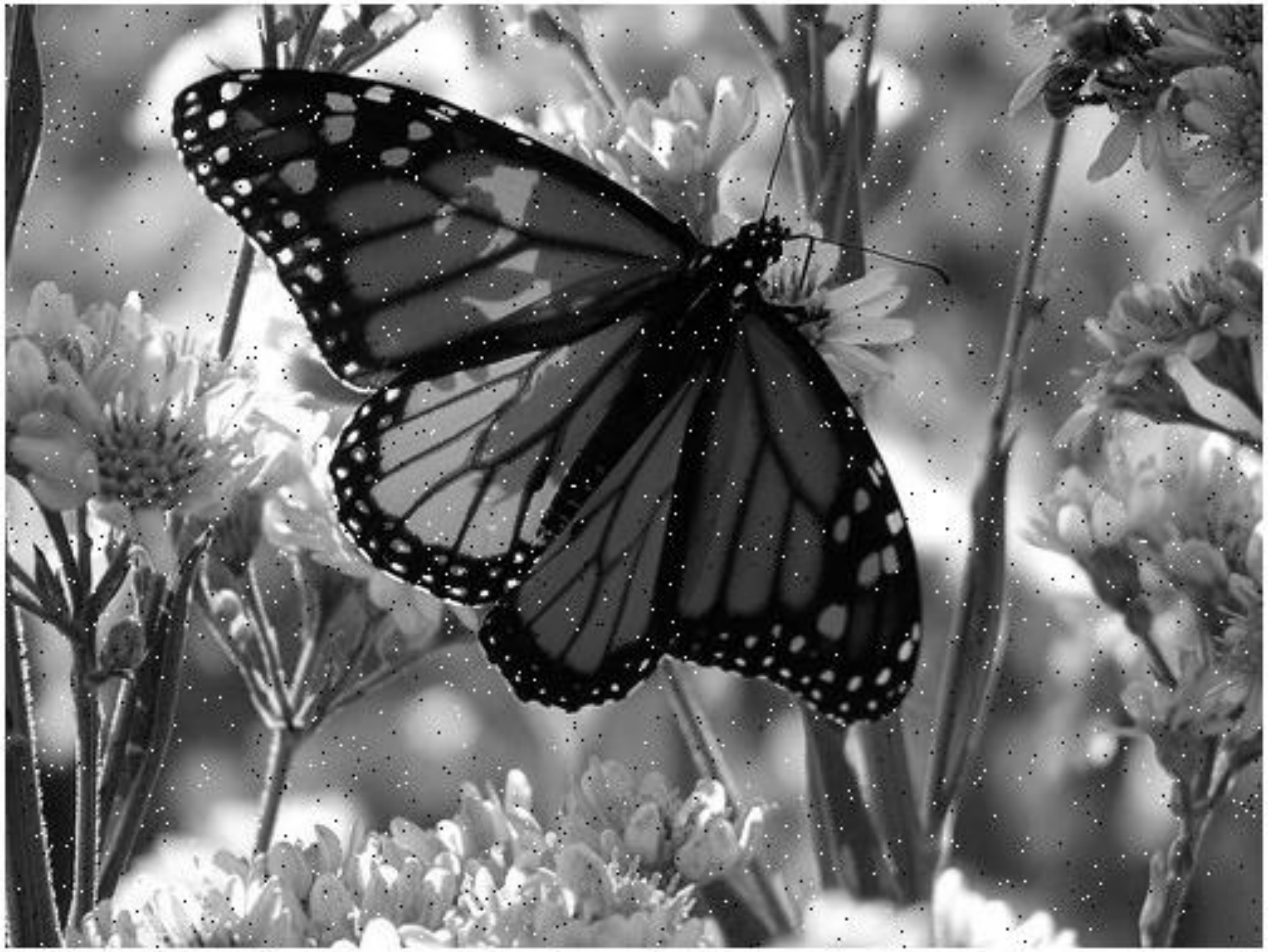
Looks like the discrete cosine bases of JPG!...

2D Discrete Cosine Basis



http://en.wikipedia.org/wiki/Discrete_cosine_transform

Noisy image



Denoised image using 15 PCA components