$\LaTeX$ command declarations here.

In [1]:
```
from __future__ import division

# plotting
%matplotlib inline
from matplotlib import pyplot as plt;
import matplotlib as mpl;
from mpl_toolkits.mplot3d import Axes3D

# scientific
import numpy as np;
import sklearn as skl;
import sklearn.datasets;
import sklearn.cluster;
import sklearn.mixture;

# ipython
import IPython;

# python
import os;
import random;

##########################################################

# image processing
import PIL;

# trim and scale images
def trim(im, percent=100):
    print("trim:", percent);
    bg = PIL.Image.new(im.mode, im.size, im.getpixel((0,0)))
    diff = PIL.ImageChops.difference(im, bg)
    diff = PIL.ImageChops.add(diff, diff, 2.0, -100)
    bbox = diff.getbbox()
    if bbox:
        x = im.crop(bbox)
        return x.resize(((x.size[0]*percent)//100,
                         (x.size[1]*percent)//100),
                        PIL.Image.ANTIALIAS);
```

EECS 445: Machine Learning

Lecture 14: Unsupervised Learning: PCA and Clustering

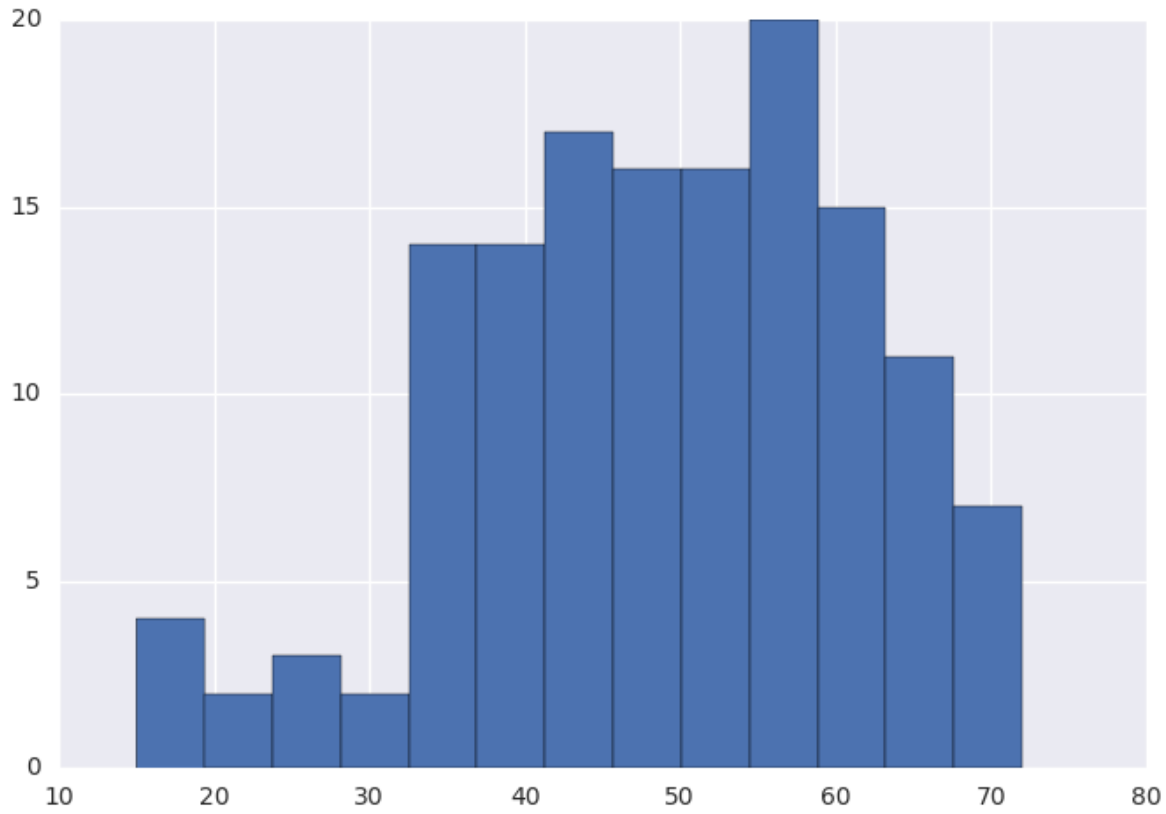
- Instructor: **Jacob Abernethy**
- Date: November 2, 2016

Midterm exam information

Statistics:

	Total Score
count	141.0
mean	48.7
std	12.4
min	15.0
25%	40.0
50%	50.0
75%	58.0
max	72.0

Score histogram



Announcements

- We will be updating the HW4 to give you all an extra week
- We will add a "free form" ML challenge via Kaggle as well
- Want a regrade on the midterm? We'll post a policy soon.

References

- **[MLAPP]** Murphy, Kevin. *Machine Learning: A Probabilistic Perspective* (https://mitpress.mit.edu/books/machine-learning-0). 2012.
- **[PRML]** Bishop, Christopher. *Pattern Recognition and Machine Learning* (http://research.microsoft.com/en-us/um/people/cmbishop/prml/). 2006.

Goal Today: Methods for *Unsupervised* Learning

We generally a call a problem "Unsupervised" when we don't have any labels!

Outline

- Principle Component Analysis
  - Classical View
  - Low dimensional representation of data
  - Relationship to SVD
- Clustering
  - Core idea behind clustering
  - K-means algorithm
  - K-means++ etc.

Principal Components Analysis

> Uses material from **[MLAPP]** and **[PRML]**

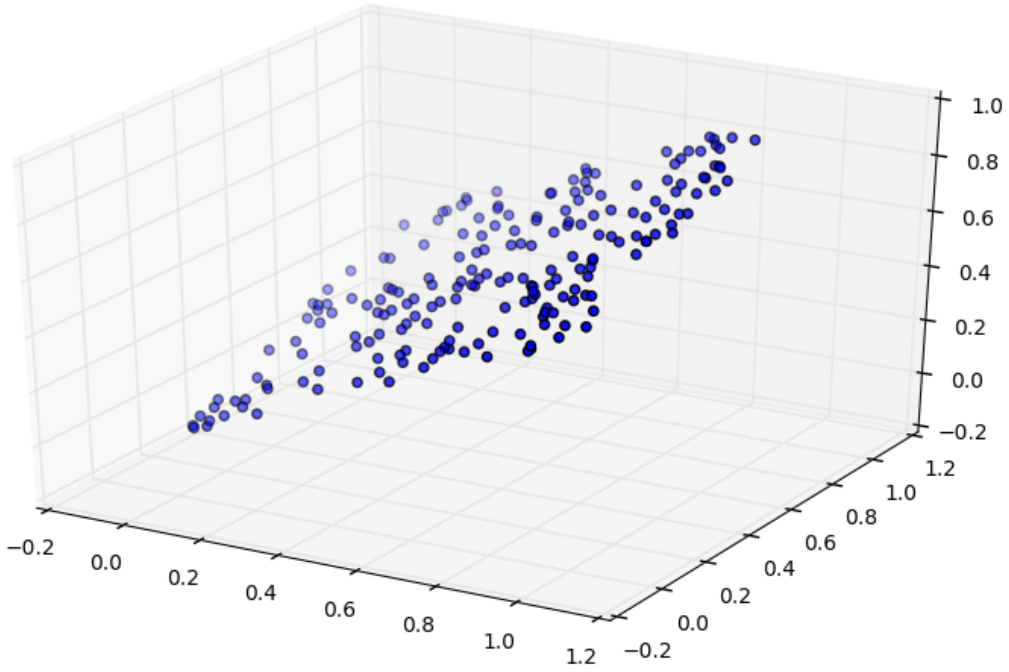
Dimensionality Reduction

High-dimensional data may have **low-dimensional structure**.

- We only need two dimensions to describe a rotated plane in 3d!

In [2]:
```
def plot_plane():
    # random samples
    n = 200;
    data = np.random.random((3,n));
    data[2,:] = 0.4 * data[1,:] + 0.6 * data[0,:];

    # plot plane
    fig = plt.figure(figsize=(10,6));
    ax = fig.add_subplot(111, projection="3d");
    ax.scatter(*data);
```

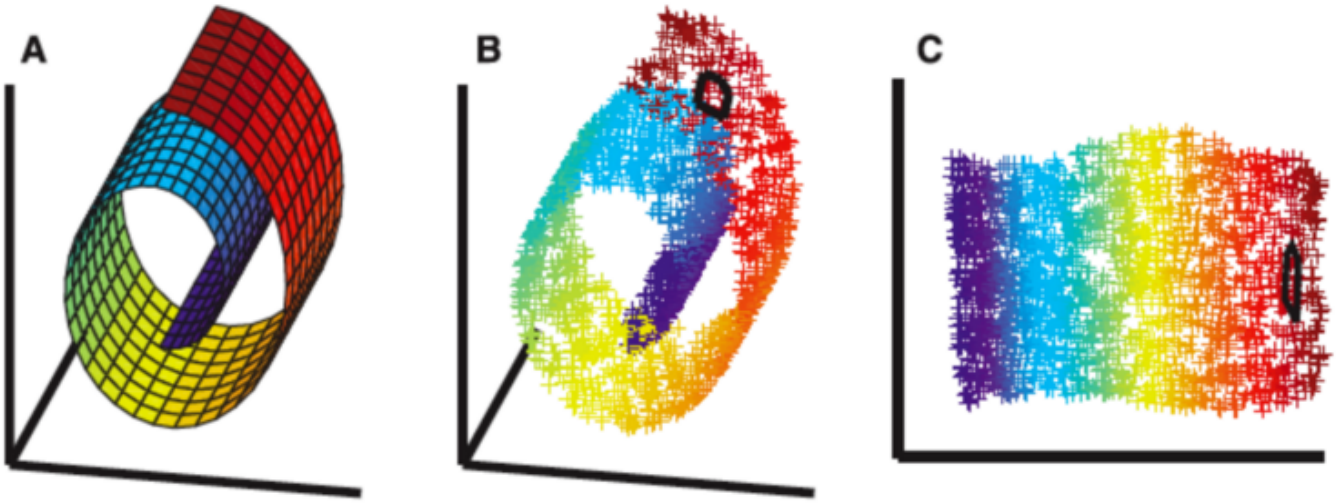
```
In [3]: plot_plane()
```



Dimensionality Reduction

Data may even be embedded in a low-dimensional **nonlinear manifold**.

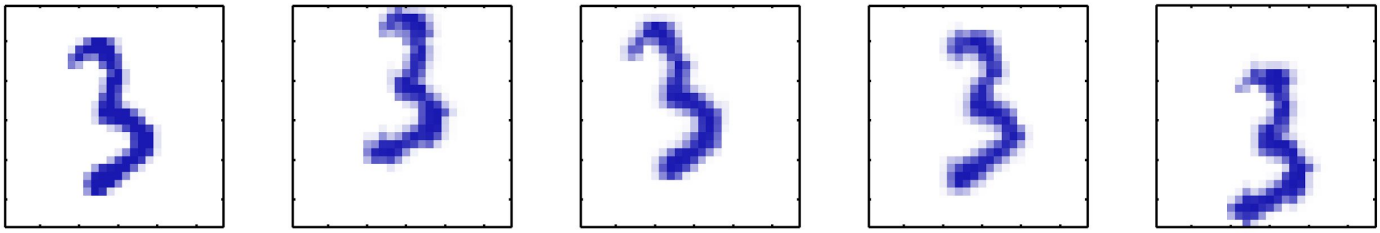
- How can we recover a low-dimensional representation?



Dimensionality Reduction

As an even more extreme example, consider a dataset consisting of the same image translated and rotate in different directions:

- Only 3 degrees of freedom for a 100x100-dimensional dataset!



Principal Components Analysis

Given a set $\boldsymbol{X} = \{\boldsymbol{x_n}\}$ of observations

- in a space of dimension $\boldsymbol{D}$,
- find a **linear subspace** of dimension $\boldsymbol{M < D}$
- that captures most of its variability.

PCA can be described in two equivalent ways:

- maximizing the variance of the projection, or
- minimizing the squared approximation error.

PCA: Equivalent Descriptions

Maximize variance or minimize squared projection error:

PCA: Equivalent Descriptions

With mean at the origin $\boldsymbol{c_i^2 = a_i^2 + b_i^2}$, with constant $\boldsymbol{c_i^2}$

- Minimizing $\boldsymbol{b_i^2}$ maximizes $\boldsymbol{a_i^2}$ and vice versa

PCA: First Principal Component

Given data points $\{x_n\}$ in D-dim space.

- Mean $\bar{x} = \frac{1}{N} \sum_{n=1}^{N} x_n$
- Data covariance ($D \times D$ matrix): $S = \frac{1}{N} \sum_{n=1}^{N} (x_n - \bar{x})(x_n - \bar{x})^T$

Let u_1 be the **principal component** we want.

- Unit length $u_1^T u_1 = 1$
- Projection of x_n is $u_1^T x_n$

PCA: First Principal Component

Goal: Maximize the projection variance over directions u_1:

$$\frac{1}{N} \sum_{n=1}^{N} \{u_1^T x_n - u_1^T \bar{x}\}^2 = u_1^T S u_1$$

- Use a Lagrange multiplier to enforce $u_1^T u_1 = 1$
  - Maximize: $u_1^T S u_1 + \lambda(1 - u_1^T u_1)$
- Derivative is zero when $S u_1 = \lambda u_1$
  - That is, $u_1^T S u_1 = \lambda$
- So u_1 is eigenvector of S with largest eigenvalue.

PCA: Maximizing Variance

The top M eigenvectors of the empirical covariance matrix S give the M principal components of the data.

- Minimizes squared projection error
- Maximizes projection variances

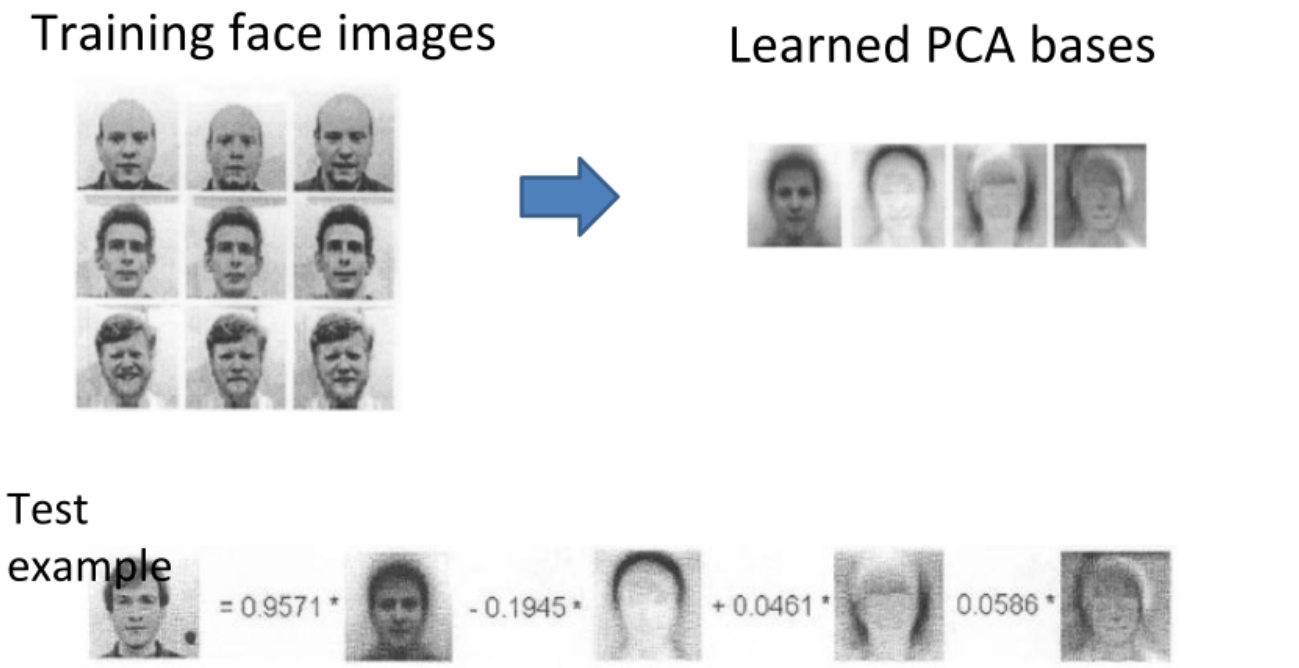
Recall: These are the top M left singular vectors of the data matrix $\hat{X}$, where $\hat{X} := X - \bar{x} 1_N$, i.e. we shift X to ensure 0-mean rows.

Key points for computing SVD

Let $\boldsymbol{X}$ be the $\boldsymbol{n} \times \boldsymbol{m}$ data matrix ($\boldsymbol{n}$ rows, one for each example). We want to represent our data using only the top $\boldsymbol{k}$ principle components.

1. Mean-center the data, so that $\bar{\boldsymbol{X}}$ is $\boldsymbol{X}$ with each row subtracted by the mean row $\frac{1}{n}\sum_i \boldsymbol{X}_{i:}$
2. Compute the SVD of $\bar{\boldsymbol{X}}$, i.e. $\bar{\boldsymbol{X}} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top$
3. We can construct $\boldsymbol{\Sigma}_{\boldsymbol{k}}$ which drops all but the top $\boldsymbol{k}$ singular values from $\boldsymbol{\Sigma}$
4. We can represent $\bar{\boldsymbol{X}}$ either in terms of the principle components, $\boldsymbol{\Sigma}_{\boldsymbol{k}}\boldsymbol{V}^\top$ or we can look at the data in the original representation after dropping the lower components, which is $\boldsymbol{U}\boldsymbol{\Sigma}_{\boldsymbol{k}}\boldsymbol{V}^\top$

Example: Eigenfaces



Images from www.cse.unr.edu/~bebis/CS485/Lectures/Eigenfaces.ppt

Example: Face Recognition via Eigenfaces

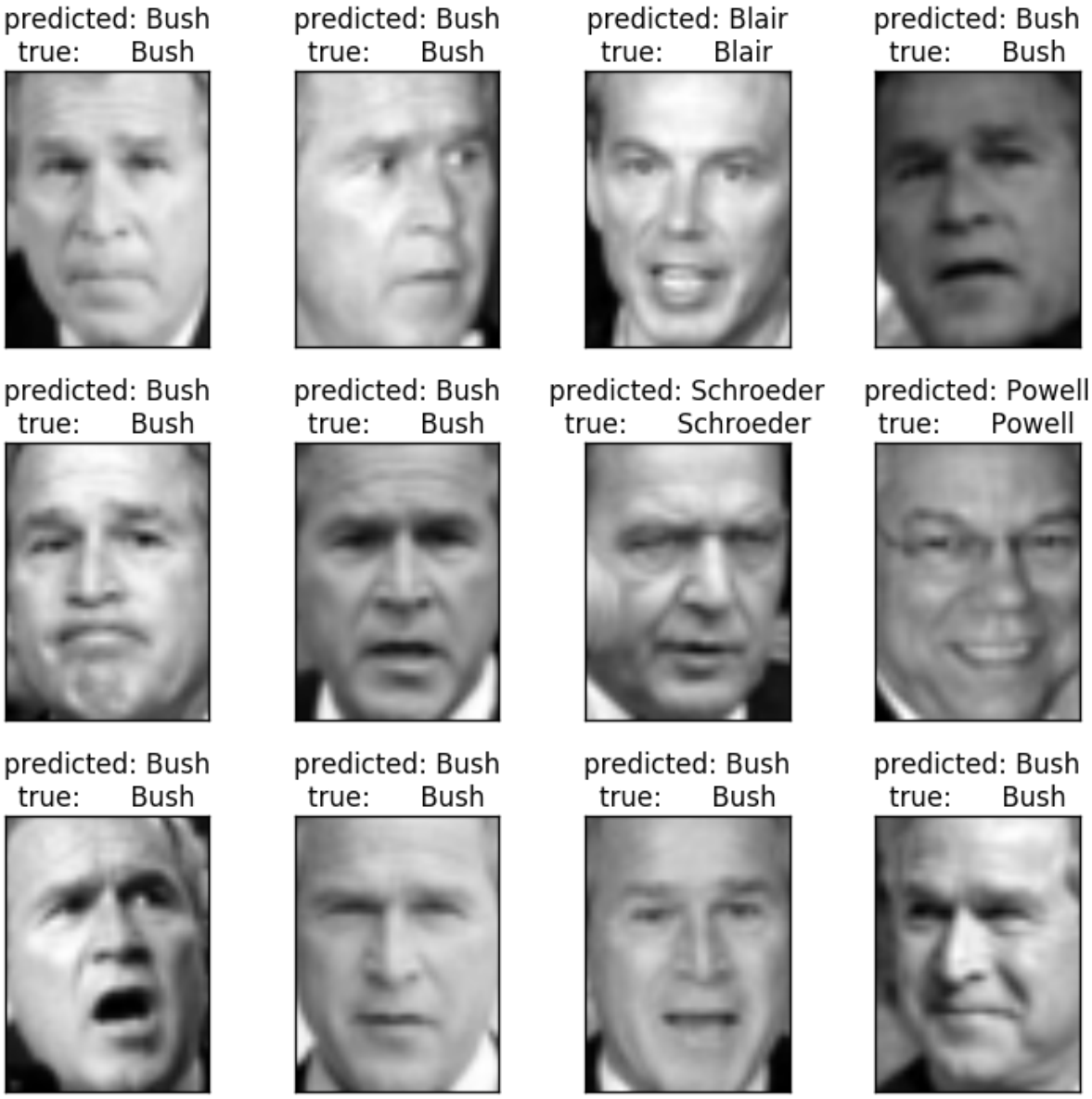
In [4]:

```
## scikit example: Faces recognition example using eigenfaces and SVMs

from __future__ import print_function

from time import time
import matplotlib.pyplot as plt

from sklearn.cross_validation import train_test_split
from sklearn.datasets import fetch_lfw_people
from sklearn.grid_search import GridSearchCV
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix
from sklearn.decomposition import RandomizedPCA
from sklearn.svm import SVC


###############################################################################
# Download the data, if not already on disk and load it as numpy arrays

lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)

# introspect the images arrays to find the shapes (for plotting)
n_samples, h, w = lfw_people.images.shape

# for machine learning we use the 2 data directly (as relative pixel
# positions info is ignored by this model)
X = lfw_people.data
n_features = X.shape[1]

# the label to predict is the id of the person
y = lfw_people.target
target_names = lfw_people.target_names
n_classes = target_names.shape[0]


###############################################################################
# Split into a training set and a test set using a stratified k fold

# split into a training and testing set
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.25, random_state=42)


###############################################################################
# Compute a PCA (eigenfaces) on the face dataset (treated as unlabeled
# dataset): unsupervised feature extraction / dimensionality reduction
n_components = 150

#print("Extracting the top %d eigenfaces from %d faces"
#      % (n_components, X_train.shape[0]))
#t0 = time()
pca = RandomizedPCA(n_components=n_components, whiten=True).fit(X_train)
#print("done in %0.3fs" % (time() - t0))
```

```
eigenfaces = pca.components_.reshape((n_components, h, w))

#print("Projecting the input data on the eigenfaces orthonormal basis")
#t0 = time()
X_train_pca = pca.transform(X_train)
X_test_pca = pca.transform(X_test)
#print("done in %0.3fs" % (time() - t0))


###############################################################################
# Train a SVM classification model

#print("Fitting the classifier to the training set")
#t0 = time()
param_grid = {'C': [1e3, 5e3, 1e4, 5e4, 1e5],
              'gamma': [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.1], }
clf = GridSearchCV(SVC(kernel='rbf', class_weight='balanced'), param_gri
d)
clf = clf.fit(X_train_pca, y_train)
#print("done in %0.3fs" % (time() - t0))
#print("Best estimator found by grid search:")
#print(clf.best_estimator_)


###############################################################################
# Quantitative evaluation of the model quality on the test set

#print("Predicting people's names on the test set")
#t0 = time()
y_pred = clf.predict(X_test_pca)
#print("done in %0.3fs" % (time() - t0))

#print(classification_report(y_test, y_pred, target_names=target_names))
#print(confusion_matrix(y_test, y_pred, labels=range(n_classes)))


###############################################################################
# Qualitative evaluation of the predictions using matplotlib

def plot_gallery(images, titles, h, w, n_row=3, n_col=4):
    """Helper function to plot a gallery of portraits"""
    plt.figure(figsize=(1.8 * n_col, 2.4 * n_row))
    plt.subplots_adjust(bottom=0, left=.01, right=.99, top=.90, hspace=.3

    for i in range(n_row * n_col):
        plt.subplot(n_row, n_col, i + 1)
        plt.imshow(images[i].reshape((h, w)), cmap=plt.cm.gray)
        plt.title(titles[i], size=12)
        plt.xticks(())
        plt.yticks(())


# plot the result of the prediction on a portion of the test set
```

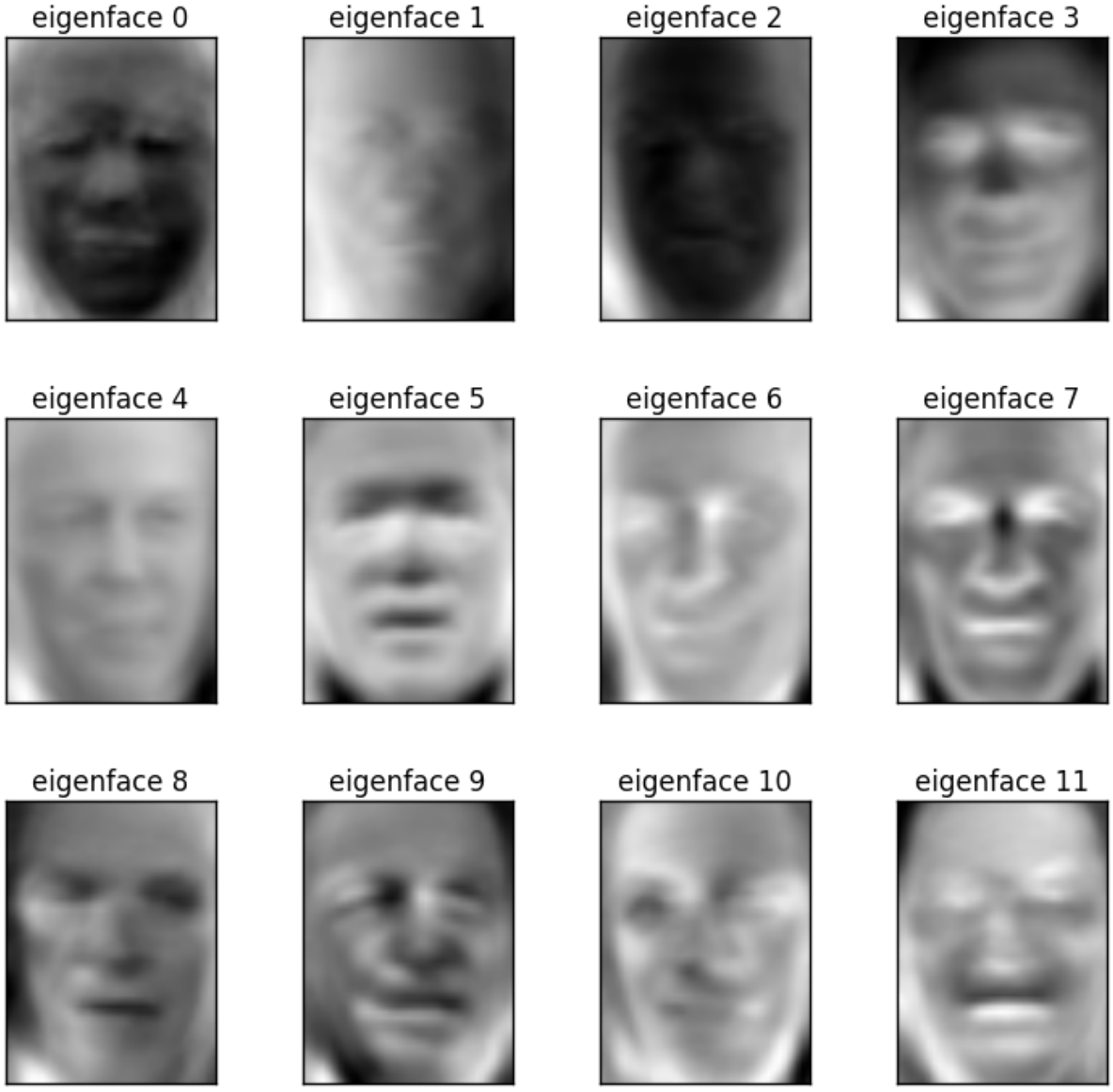
```
def title(y_pred, y_test, target_names, i):
    pred_name = target_names[y_pred[i]].rsplit(' ', 1)[-1]
    true_name = target_names[y_test[i]].rsplit(' ', 1)[-1]
    return 'predicted: %s\ntrue:      %s' % (pred_name, true_name)

prediction_titles = [title(y_pred, y_test, target_names, i)
                     for i in range(y_pred.shape[0])]
```

In [5]:
```
plot_gallery(X_test, prediction_titles, h, w)
```



Example: Face Recognition

In [6]:
```
eigenface_titles = ["eigenface %d" % i for i in
range(eigenfaces.shape[0])]
plot_gallery(eigenfaces, eigenface_titles, h, w)
```



Break time!

Soon to come: Latent Variable Models

> Uses material from **[MLAPP]** §10.1-10.4, §11.1-11.2

Latent Variable Models

In general, the goal of probabilistic modeling is to

> Use what we know to make *inferences* about what we don't know.

Graphical models provide a natural framework for this problem.

- Assume unobserved variables are correlated due to the influence of unobserved **latent variables**.
- Latent variables encode beliefs about the generative process.

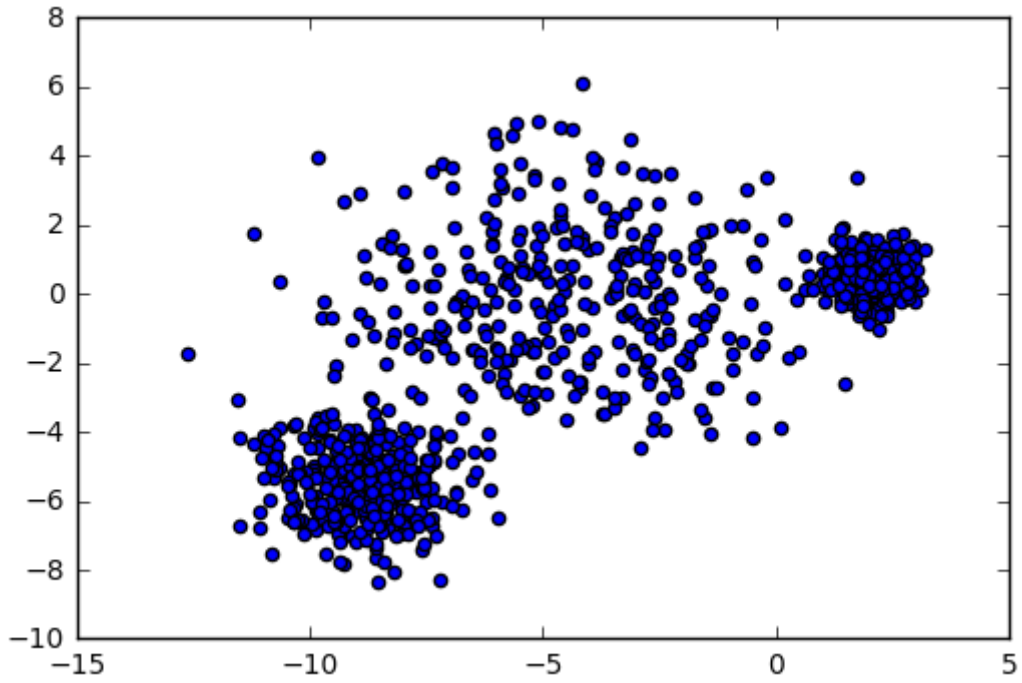
Example to Come: Gaussian Mixture Models

This dataset is hard to explain with a single distribution.

- Underlying density is complicated overall...
- But it's clearly three Gaussians!

In [7]:
```
X, y = skl.datasets.make_blobs(1000, cluster_std=[1.0, 2.5, 0.5], random
_state=170)
plt.scatter(X[:,0], X[:,1])
```

Out[7]: <matplotlib.collections.PathCollection at 0x116f79a20>



Clustering & K-Means

> Uses material from **[PRML]** §9.1

Clustering: Introduction

Goal: Partition data $\mathcal{X} = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ into K disjoint **clusters**.

- Points within a cluster should be more similar to each other than to points in other clusters.
- Estimate **cluster centers** $\mu_k \in \mathbb{R}^d$ for $k = 1, \ldots, K$
- Estimate **cluster assignments** $z_j \in \{1, \ldots, K\}$ for each point x_j

Usually, we fix K beforehand! Use model selection to overcome this limitation.

K-Means Clustering

The **K-Means** algorithm takes a simple, non-probabilistic approach.

- First, pick random cluster centers μ_k.

Then, repeat until convergence:

E-Step: Assign x_j to the nearest cluster center μ_k,

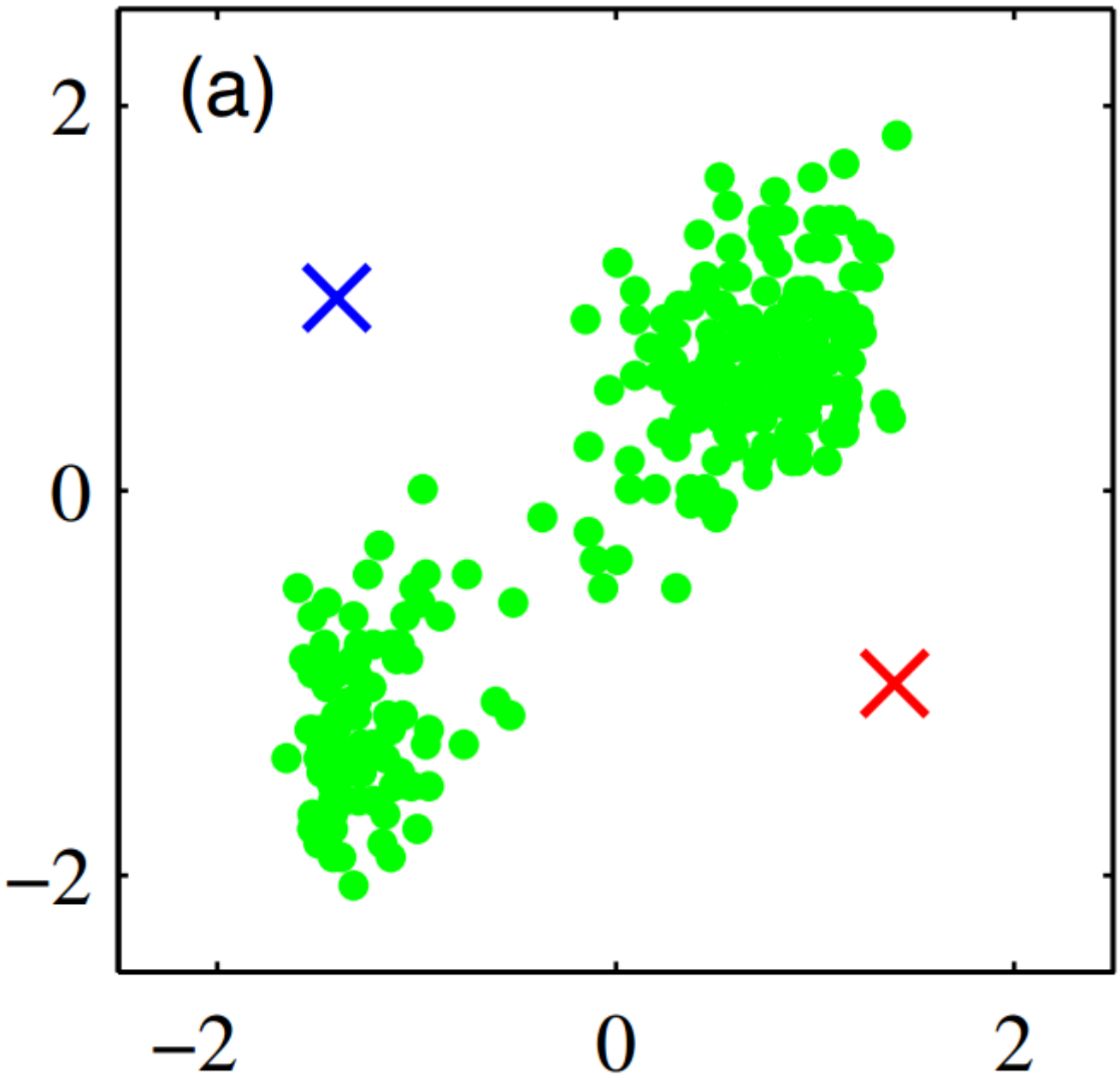
$$z_j = \arg\min_k ||x_j - \mu_k||^2$$

M-Step: Re-estimate cluster centers by averaging over assignments:

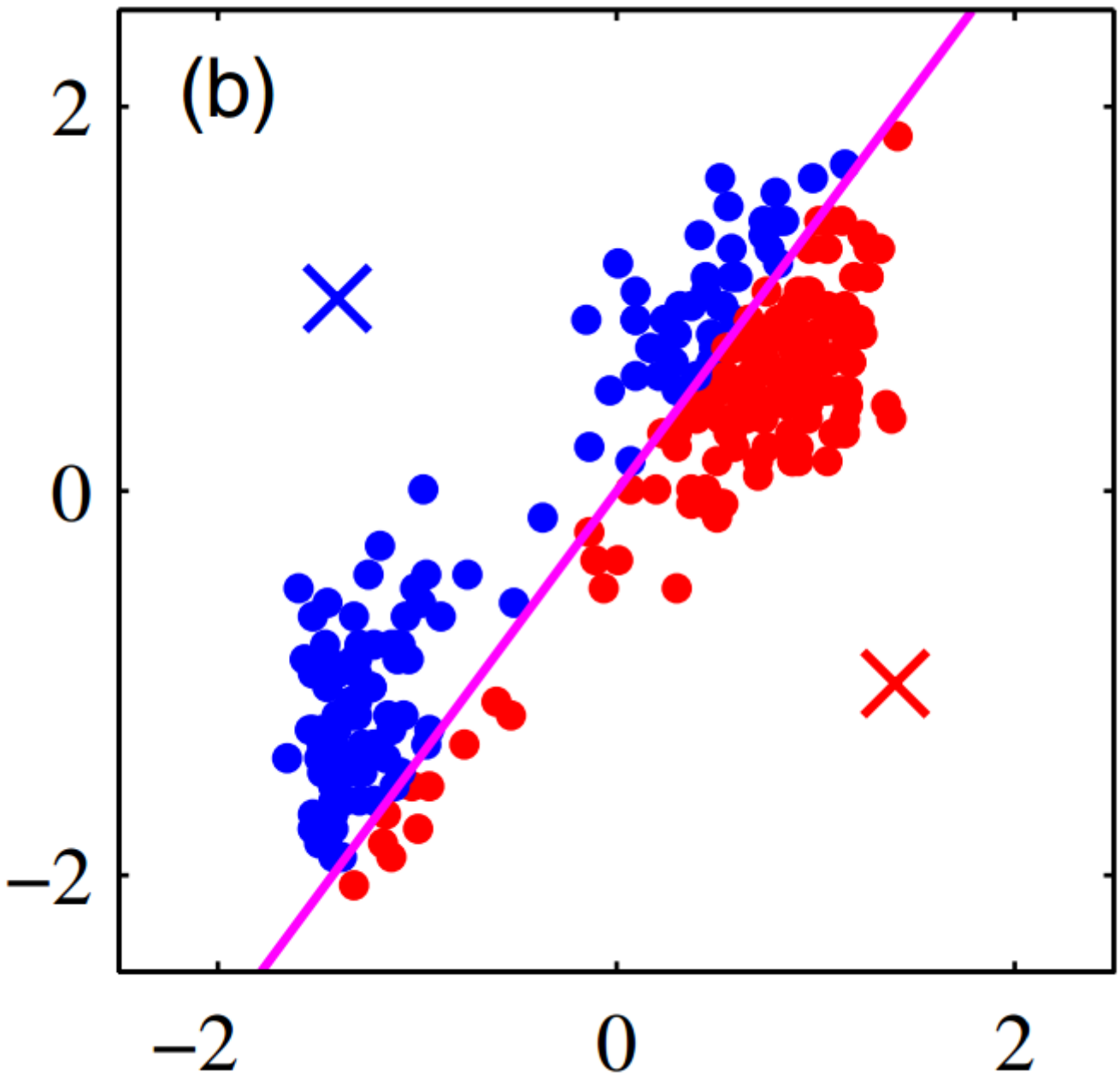
$$\mu_k = \frac{1}{\#\{j \mid z_j = k\}} \sum_{j=1}^{N} x_j \mathbb{I}(z_j = k)$$

K-Means Clustering: Initialization

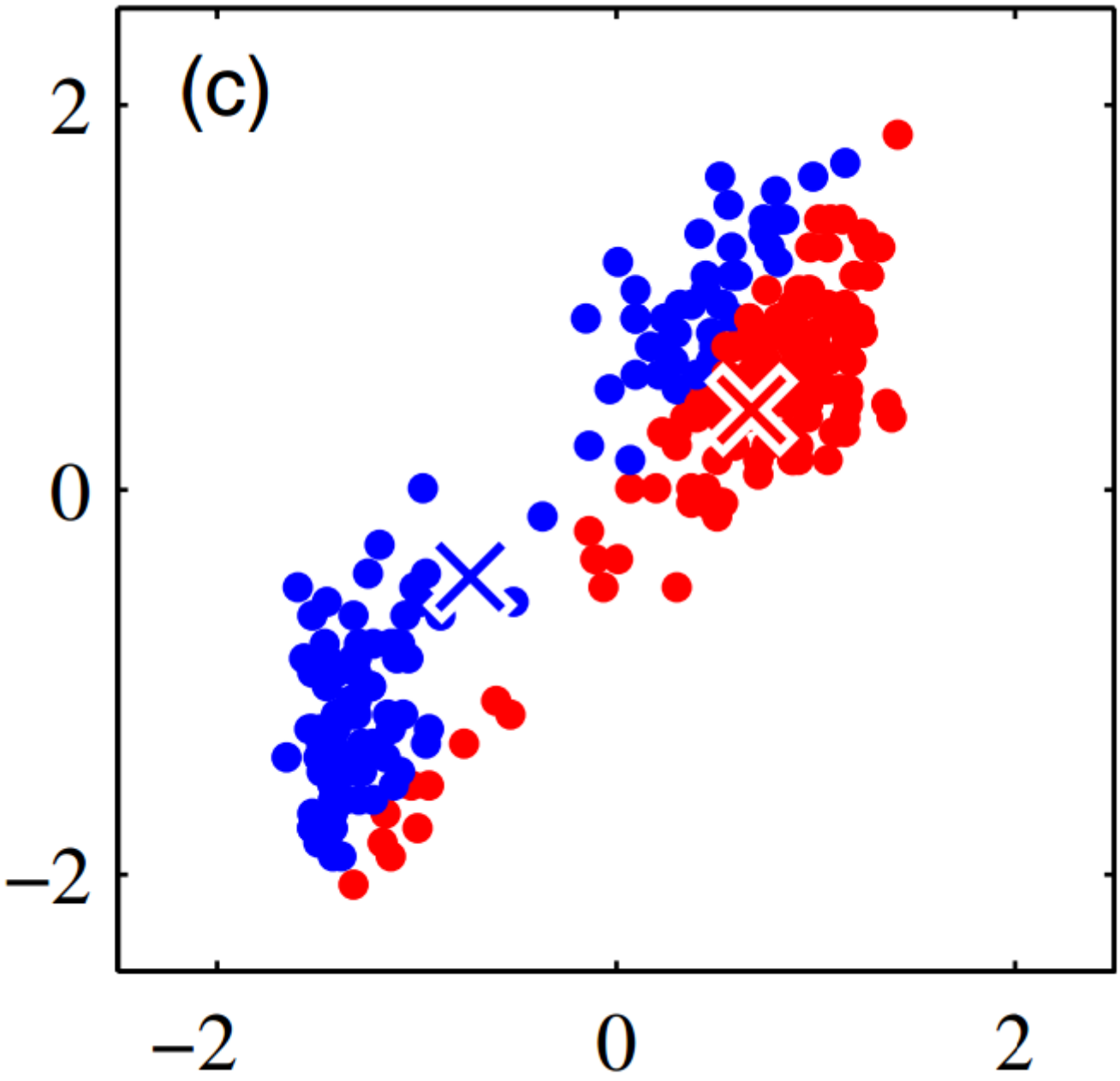
Images taken from Bishop, **[PRML]**



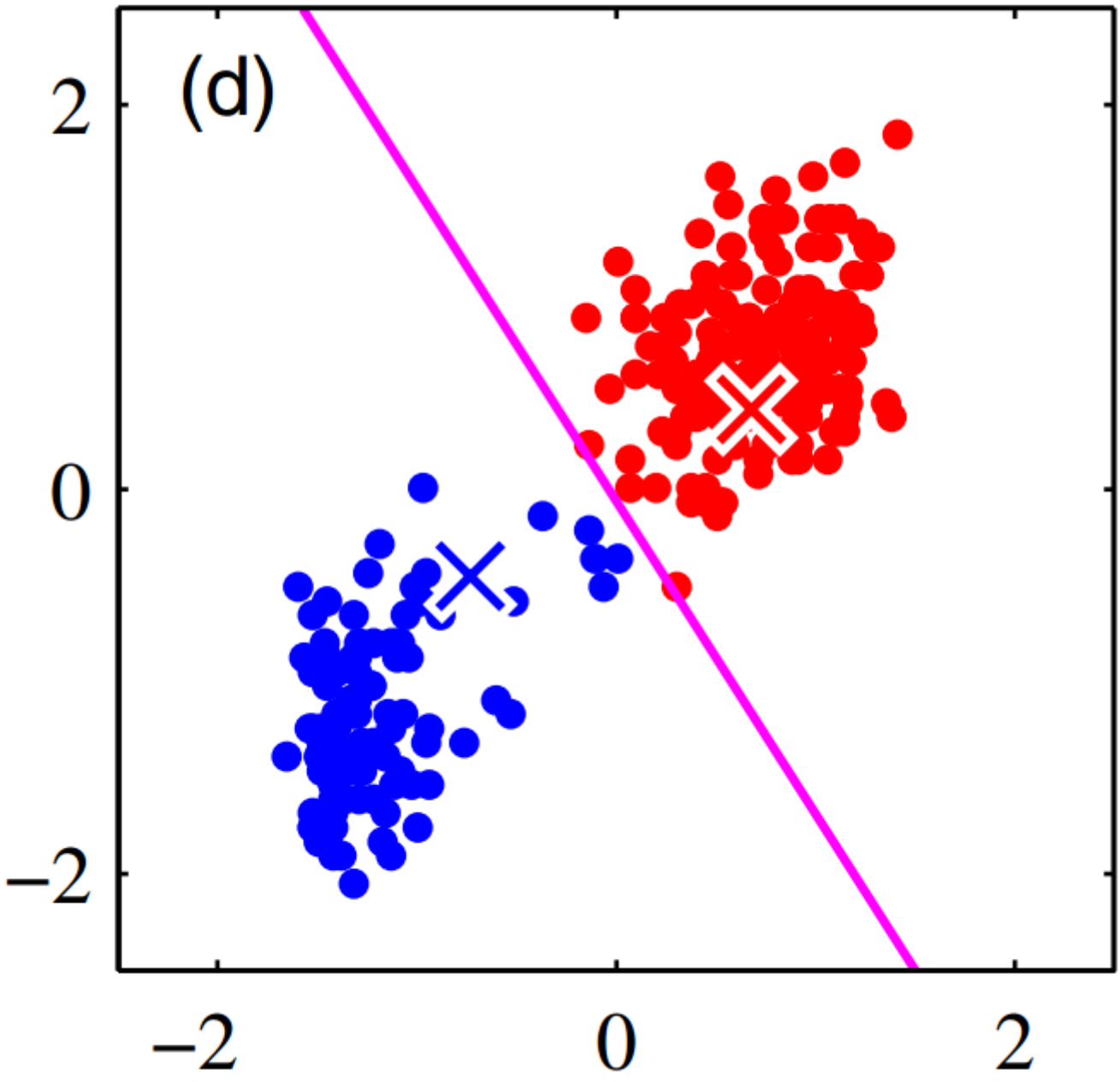
K-Means Clustering: E-Step



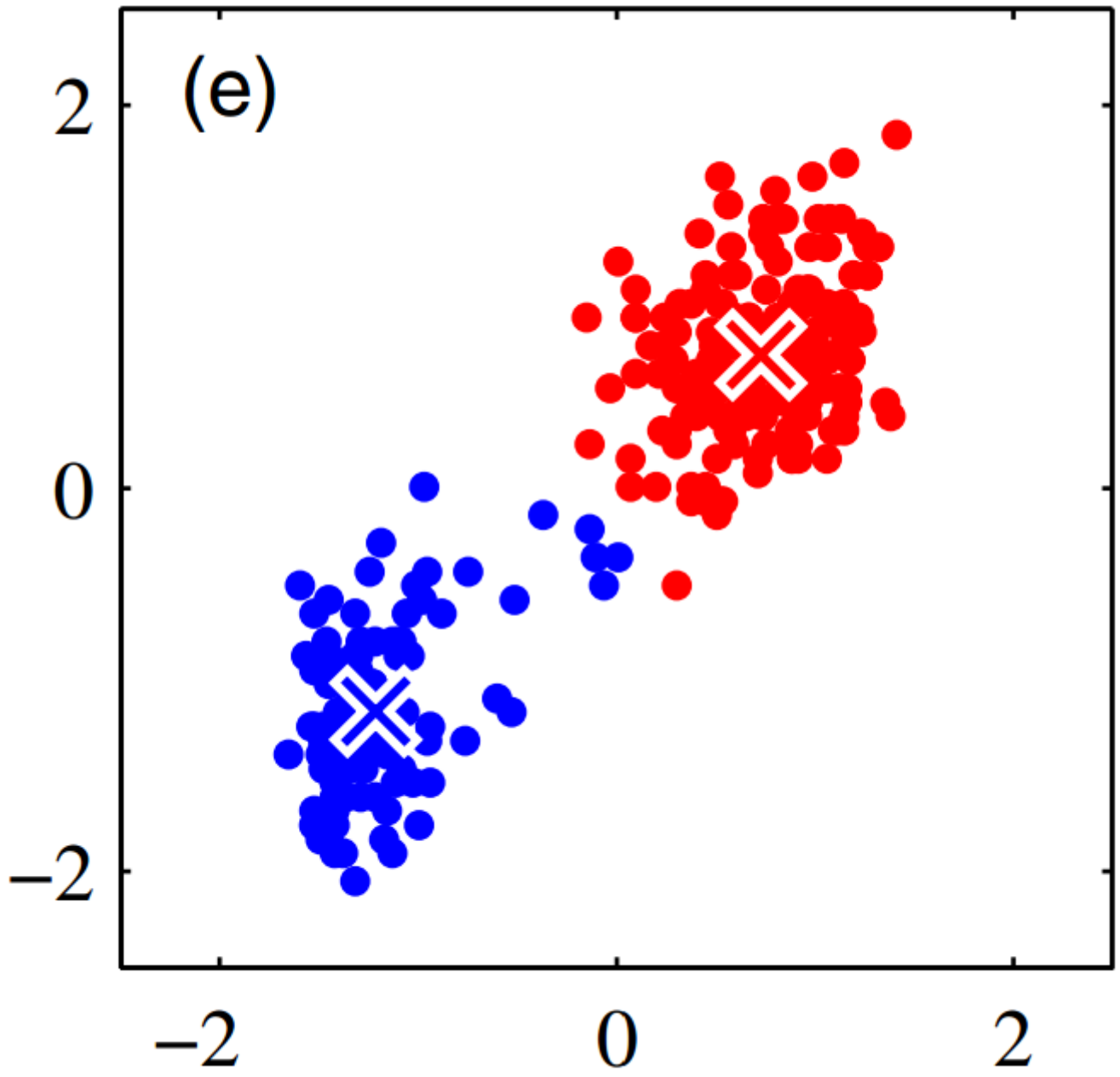
K-Means Clustering: M-Step



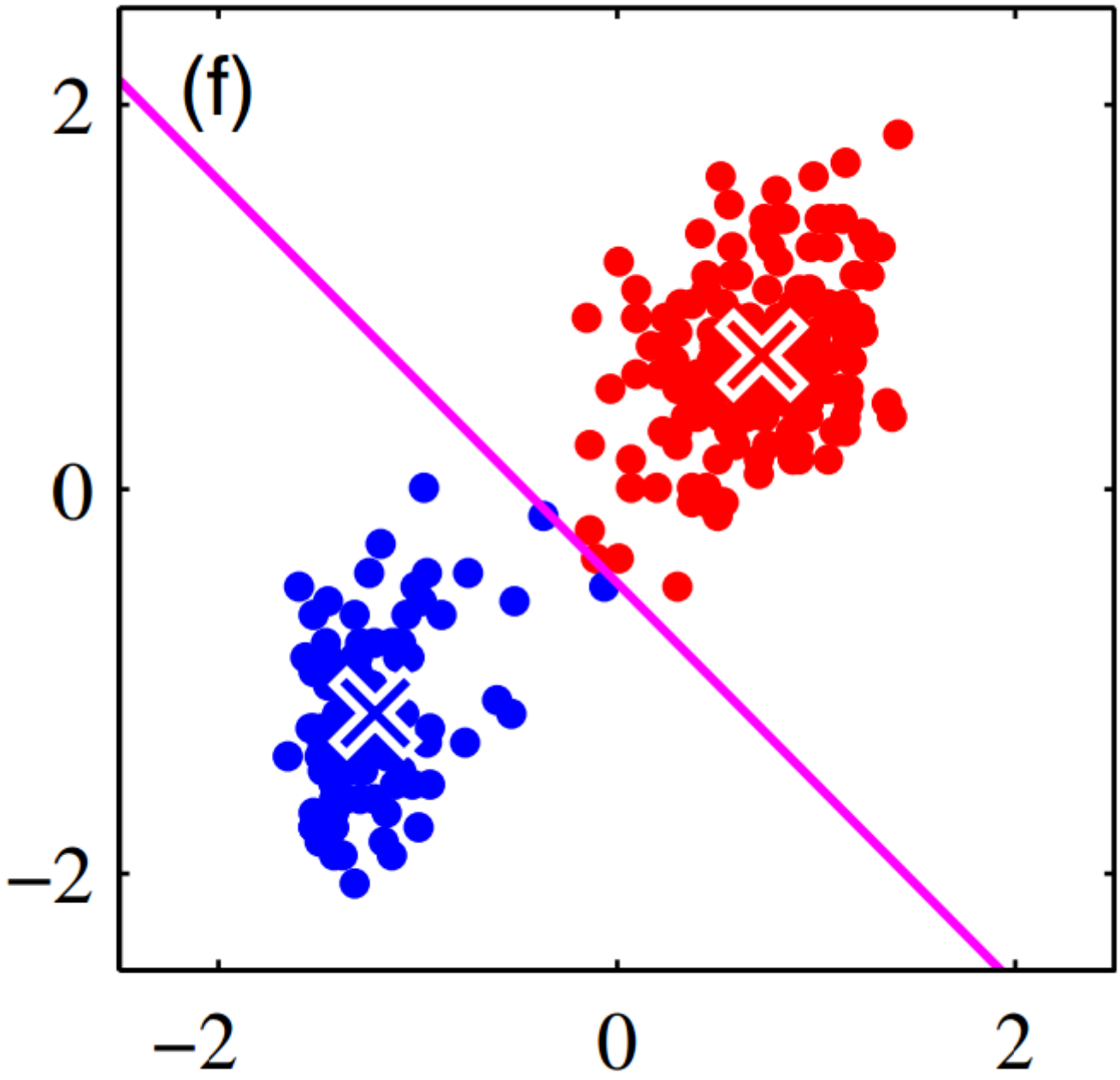
K-Means Clustering: E-Step



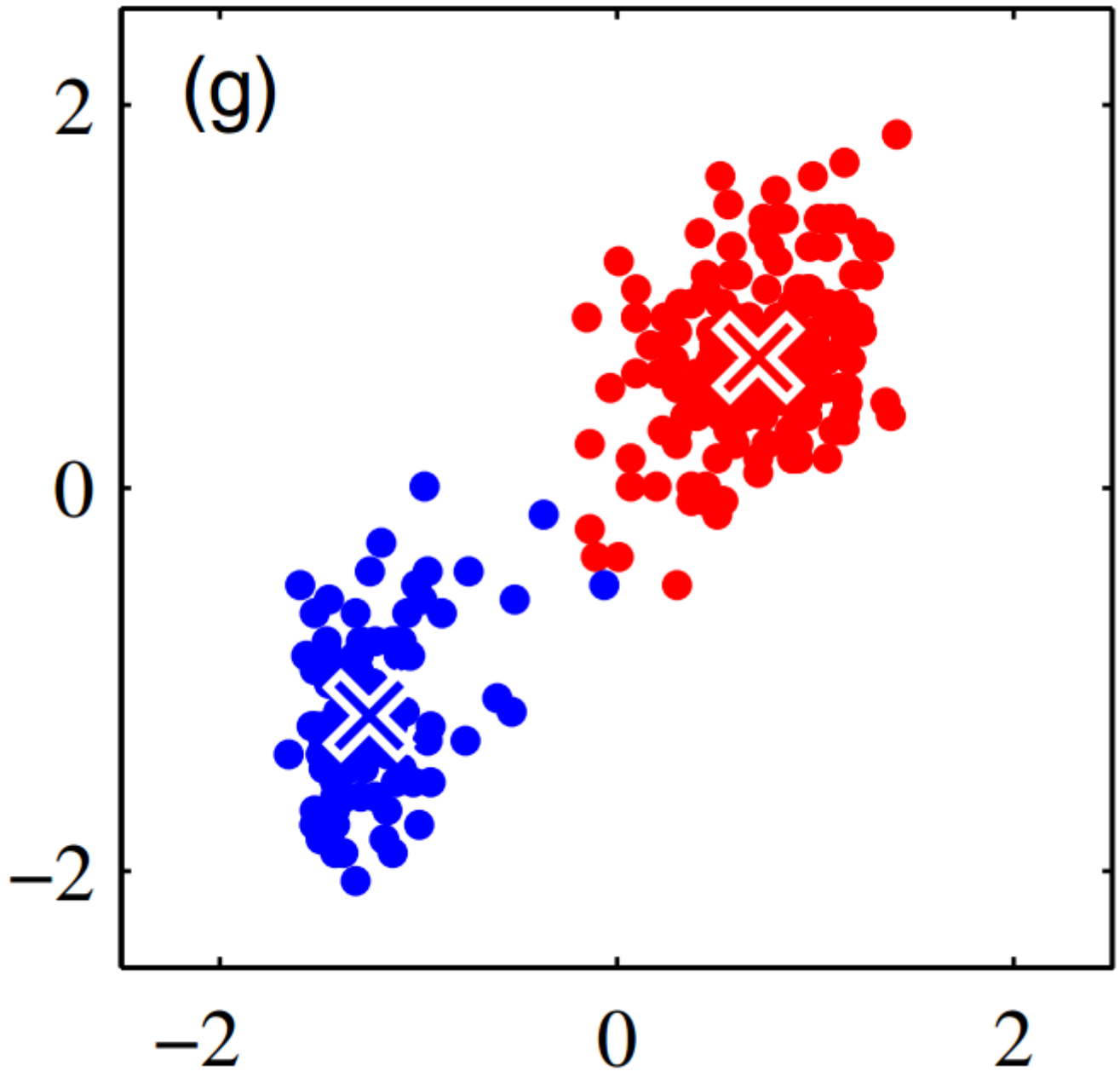
K-Means Clustering: M-Step



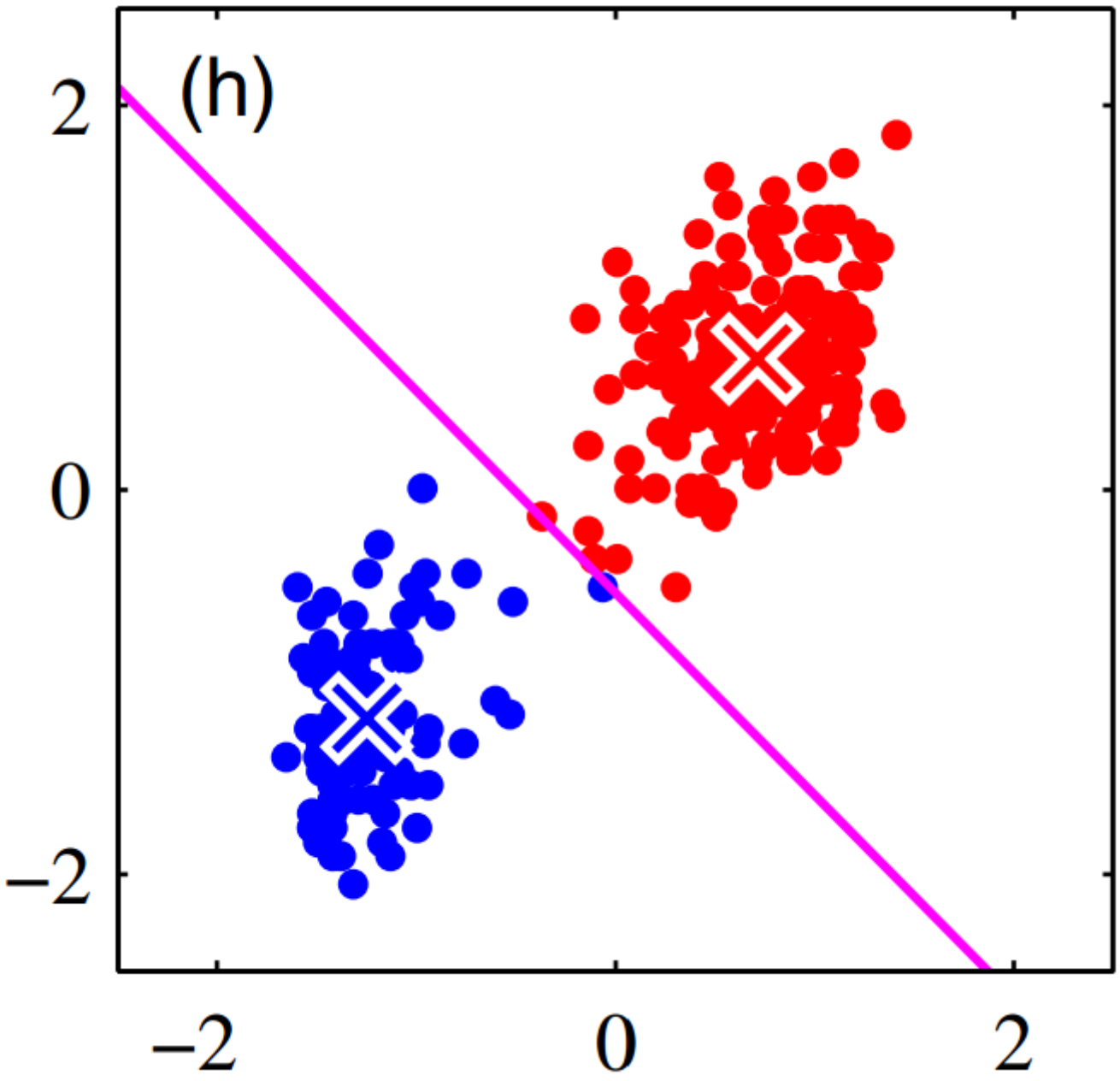
K-Means Clustering: E-Step



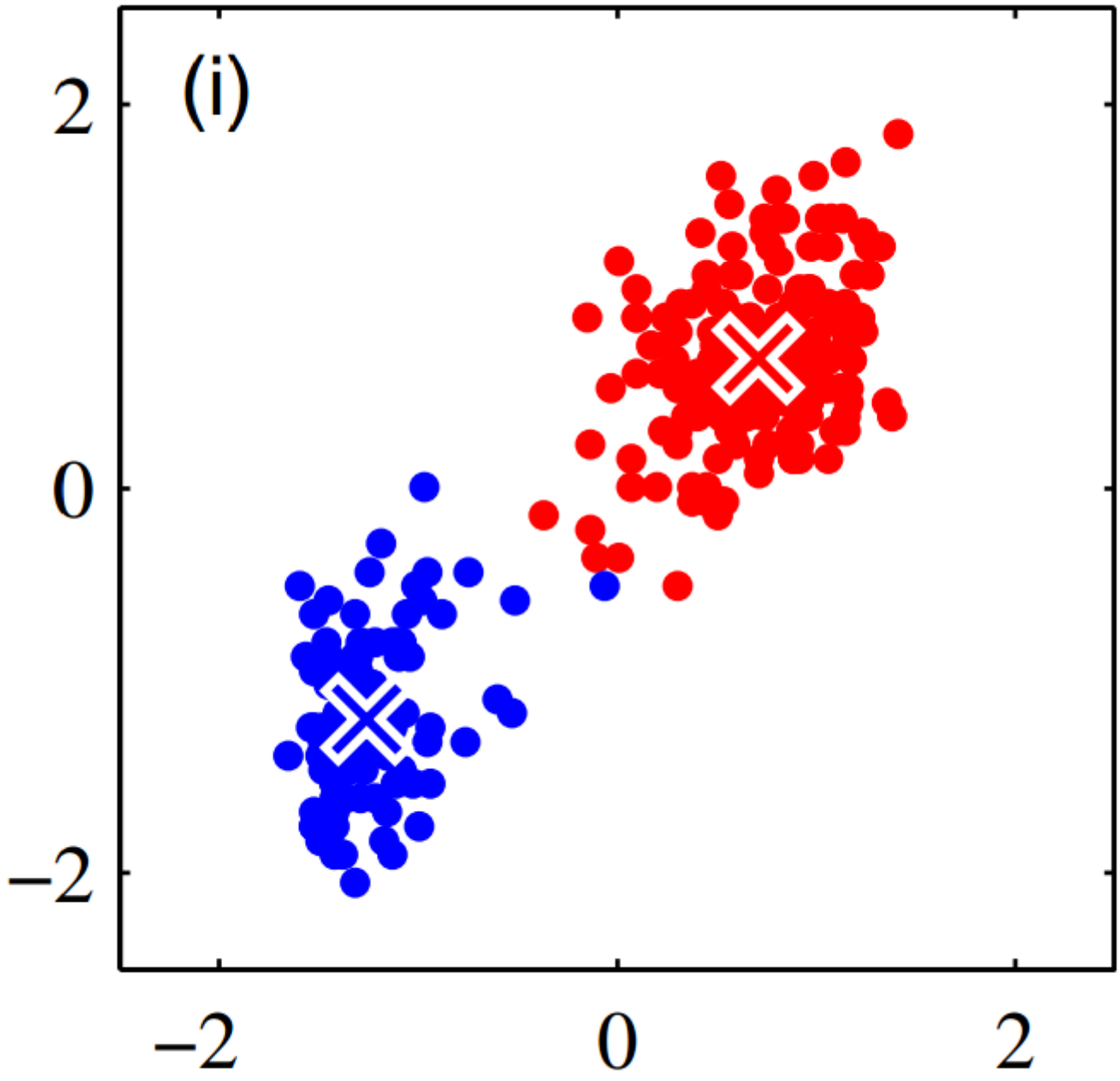
K-Means Clustering: M-Step



K-Means Clustering: E-Step



K-Means Clustering: M-Step



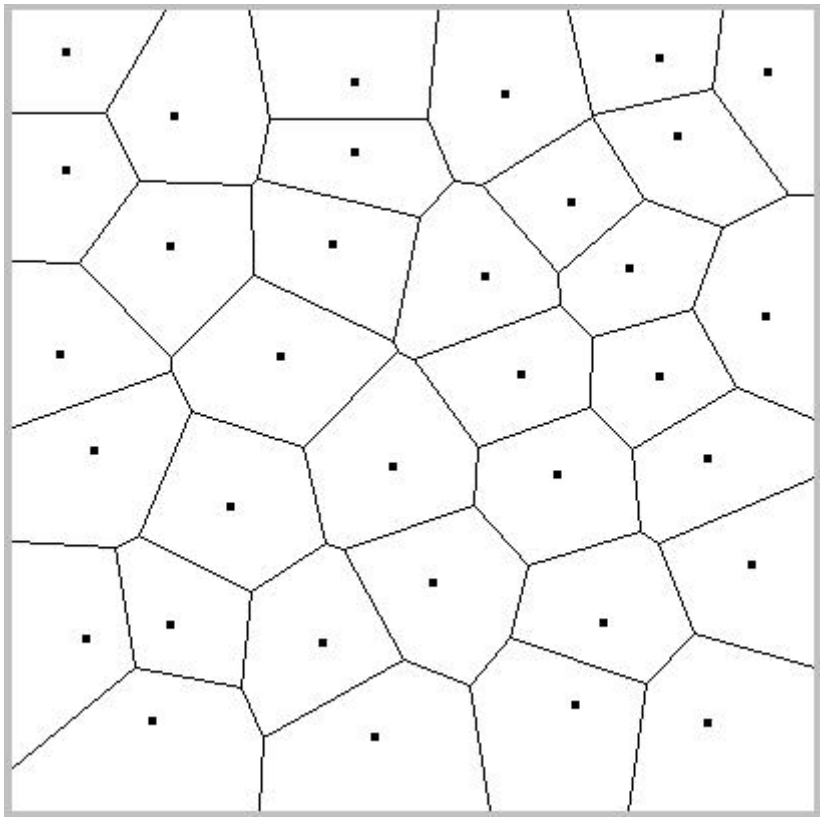
K-Means: Cluster Geometry

Clusters are convex *nearest-neighbor* regions or **Vornoi Cells**.

- Piecewise-linear boundaries

K-means will fail to identify non-convex clusters.

- However, **kernelized K-means** is possible!



K-Means Clustering: Analysis

Exercise: Show that the K-Means algorithm finds a local minimum of the **distortion measure**, given by

$$J(\mu_1, \ldots, \mu_k; z_1, \ldots, z_N) = \sum_{j=1}^{N} \sum_{k=1}^{K} \mathbb{I}(z_j = k) ||x_j - \mu_k||^2$$

K-Means: Variants

K-Means is simple and easy to extend:

- **K-Means++:** Intelligently pick initial cluster centers
- **K-Means--:** Handle outliers
- **Nonparametric K-Means:** Automatically select number of clusters
- **Kernelized K-Means:** Non-convex clusters

Next lecture, we will cover **probabilistic clustering** through the use of mixture models.

Variant: K-Means++ (http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf)

Instead of initializing cluster centers randomly,

1. Choose the first cluster center to be a random datapoint.
2. Repeat until K cluster centers have been selected:
   A. For each datapoint x_j, compute distance $D(x_j)$ to nearest cluster.
   B. Choose data point x_j at random to be the new cluster center, with probability proportional to $D(x_j)^2$.
3. Run K-means as usual.

Variant: K-Means-- (http://pmg.it.usyd.edu.au/outliers.pdf)

Vanilla K-Means is sensitive to outliers. Instead, assume there are ℓ outliers, then

1. Choose initial cluster centers as usual.
2. For $k = 1, 2, \ldots$:
   A. For each datapoint x_j, compute distance $D(x_j)$ to nearest cluster.
   B. Set L_k to be the ℓ datapoints farthest from any cluster.
   C. Perform the E and M steps as usual on $X \setminus L_k$.
3. Return most recent outlier estimate L_k in addition to usual cluster data.

Variant: Nonparametric K-Means (http://www.cs.berkeley.edu/~jordan/papers/kulis-jordan-icml12.pdf)

Automatically add new clusters via a **maximum cluster radius** λ.

1. Init $K = 1$ and set μ_1 to be the mean over datapoints.
2. Repeat until convergence:
    A. For each point x_j,
        a. Compute distance $D(x_j)$ to nearest cluster.
        b. If $D(x_j) > \lambda$, increment K and create a new cluster centered at x_j.
        c. Otherwise, assign x_j to a cluster as usual.
    B. Re-estimate cluster centers as usual.