CSCE 421: Machine Learning

Lecture 15: Principal Component Analysis and K-Means Clustering

Texas A&M University

CSCE 421

Bobak Mortazavi

Ryan King

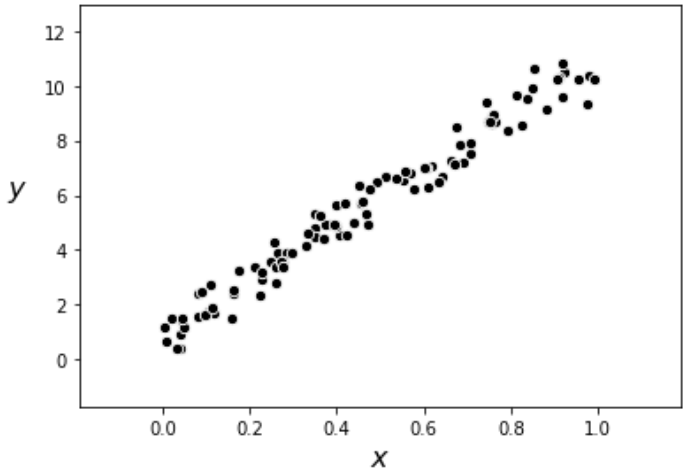
Zhale Nowroozilarki

Goals

- Understanding feature scaling and dimension reduction
- Standard normalization
- Principal component analysis
- Unsupervised Learning: Clustering via K-Means

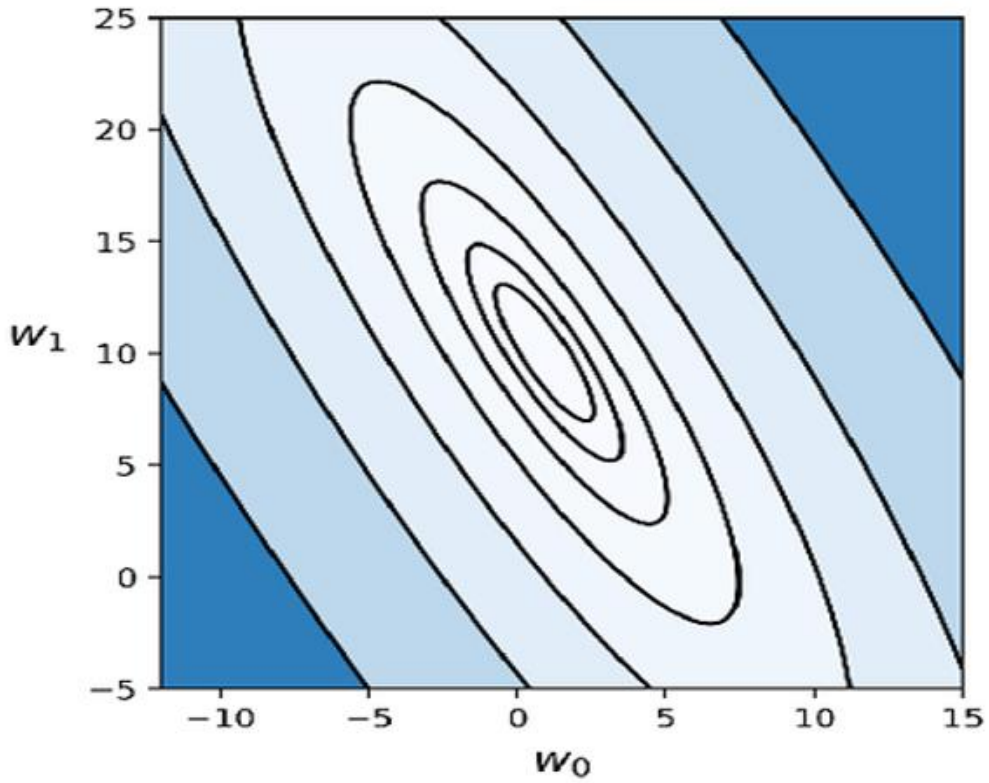
Standard Normalization of Data

- Let's assume we want to perform regression on data as in this figure
- It appears the data is roughly on a line
- Note however that the scales of x and y differ significantly



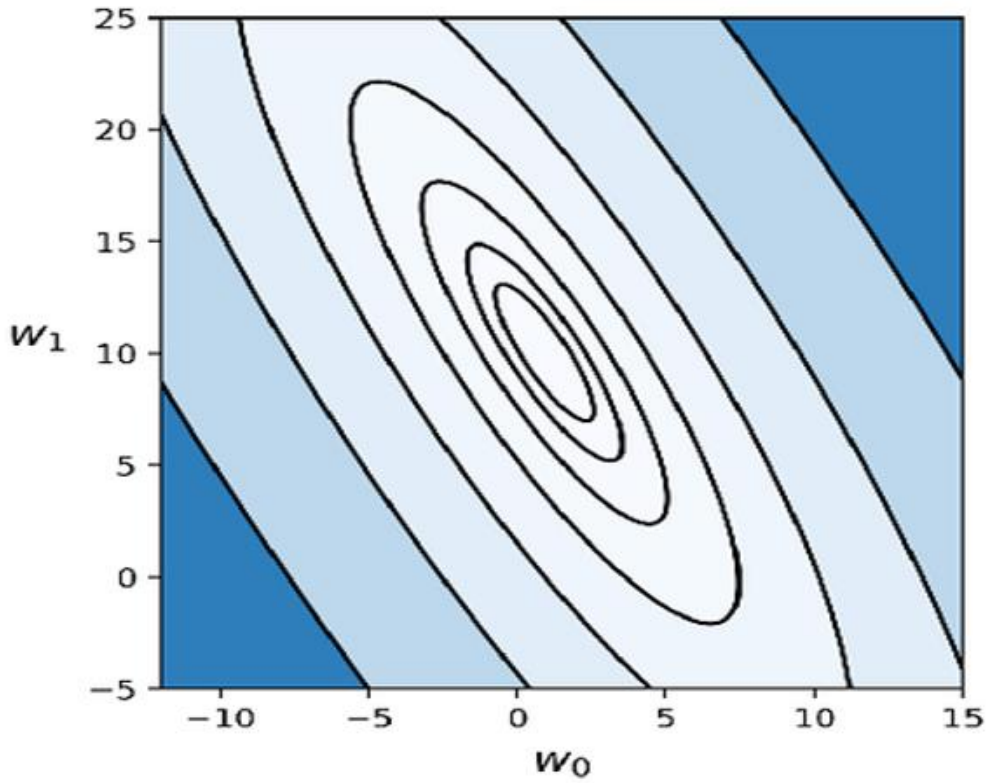
How does this impact modeling?

- If we plot the least squares cost function we see that
- The contours are elliptical
- There is a long narrow value along the axis of the ellipses



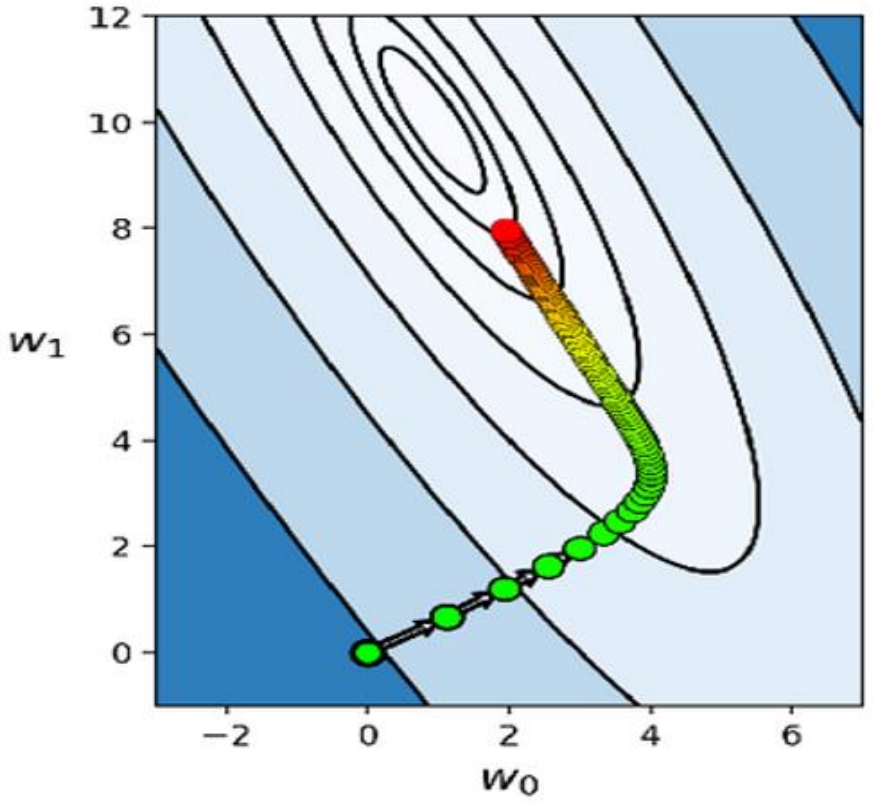
How does this impact modeling?

- If we plot the least squares cost function we see that
- The contours are elliptical
- There is a long narrow value along the axis of the ellipses
- An important question to ask:
  - How does this impact gradient descent optimization?



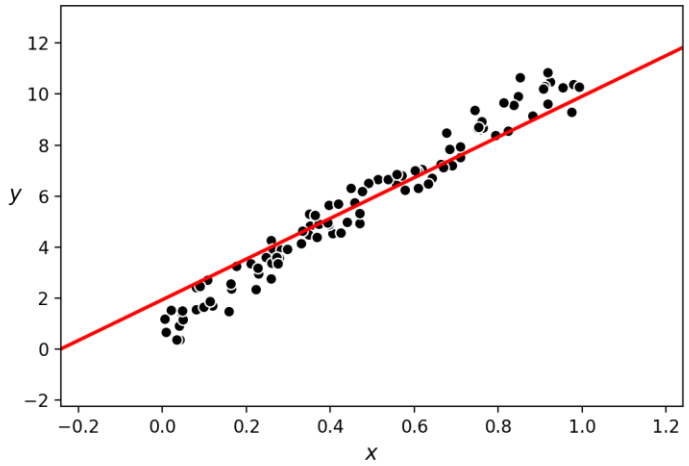
How does this impact modeling?

- If we plot the least squares cost function we see that
- The contours are elliptical
- There is a long narrow value along the axis of the ellipses
- An important question to ask:
  - How does this impact gradient descent optimization?
- They make gradient descent slow
- Unless we get lucky to initialize the algorithm along the short axis it takes gradient descent time to find that axis



Standard Normalization of Data

- Taking that solution we plot the line of best fit and see that we have a poor solution
- So, we will seek to change our shape of our least squares cost function to pave the way for more accurate and quicker gradient descent
- The adjustment we make: standard normalization



Centering and Scaling Data

- Assume for every vector x, which has p dimensions, we can scale feature p by:

$$x_p = \frac{x_p - \mu_p}{\sigma_p}$$

- Where

$$\mu_p = \frac{1}{N}\sum_{i=1}^{N} x_{pi}$$

which is the mean of the pth feature across all N subjects in the data

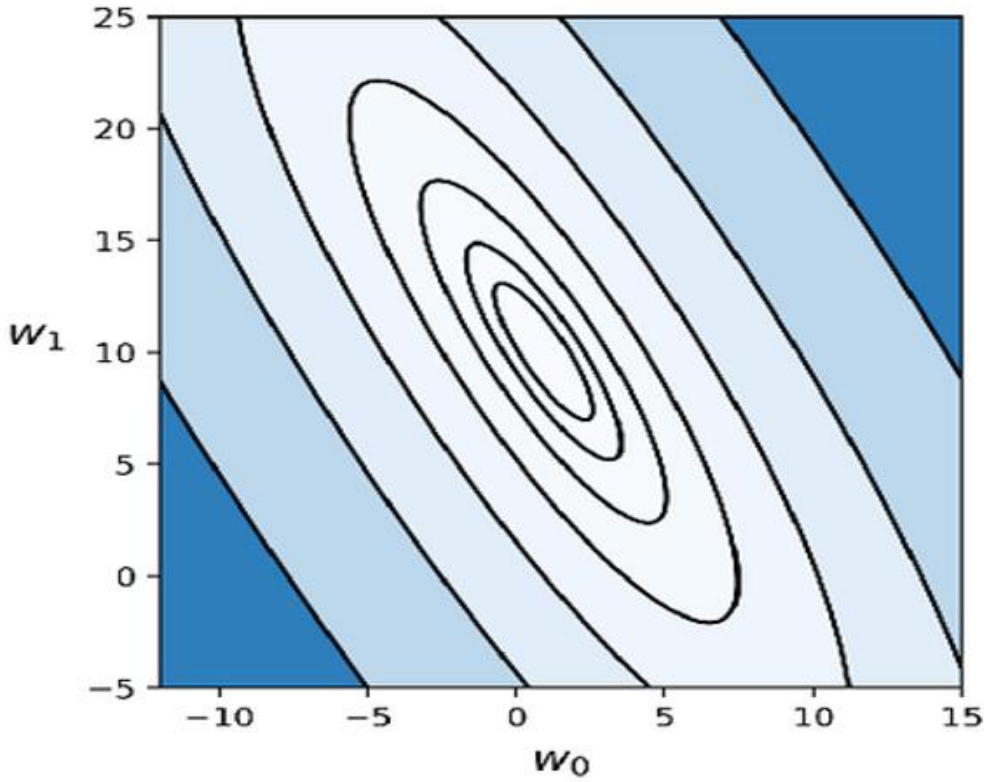
And

$$\sigma_p = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_{pi} - \mu_p)^2}$$

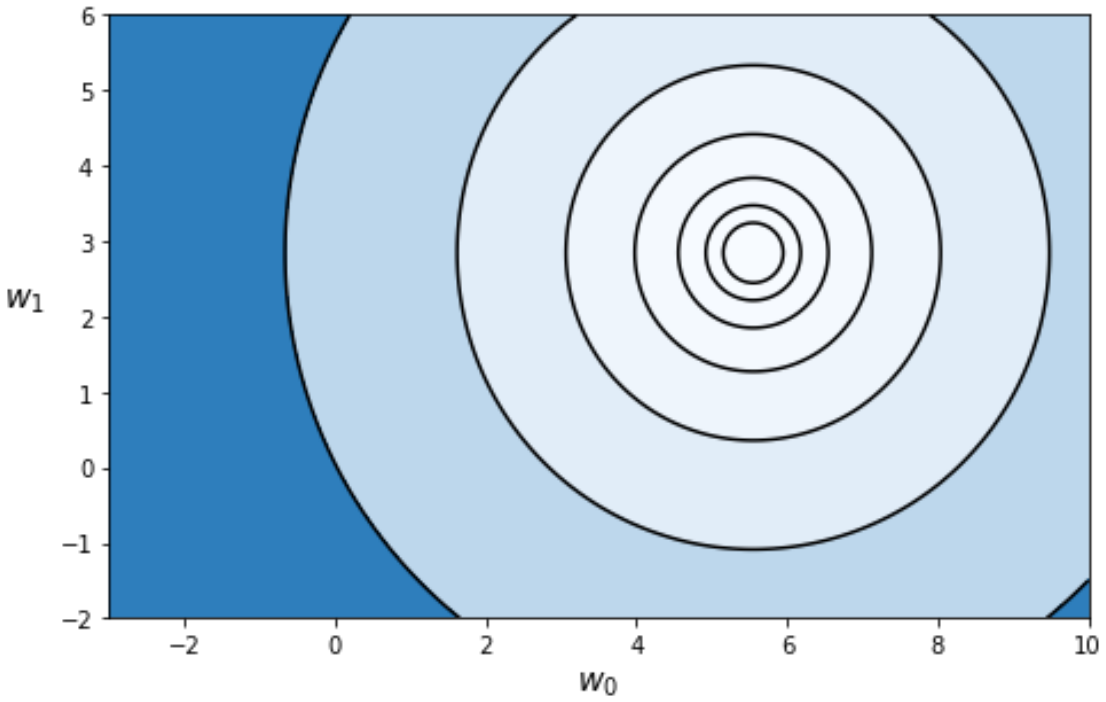
This is often called standard normalization – 0 mean and unit standard deviation for all data elements.

Revisiting our Contours

Without feature normalization

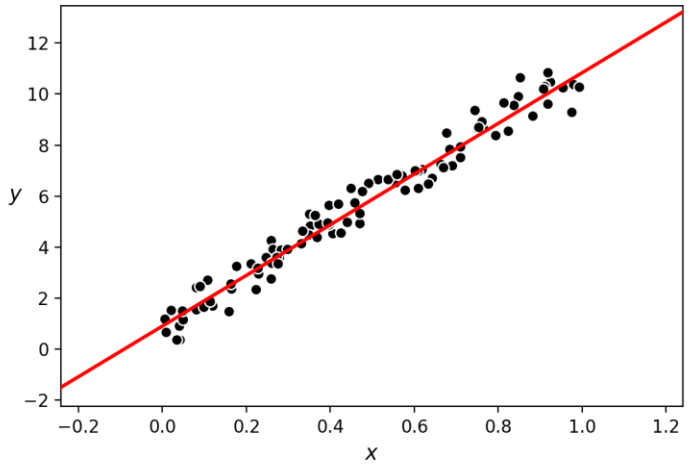


With feature normalization



Standard Normalization of Data

- With only 5 steps of gradient descent we get a much better fit line
- We have to be careful if our denominator is 0 for any specific feature
- Can apply this across all features x



Principal Component Analysis

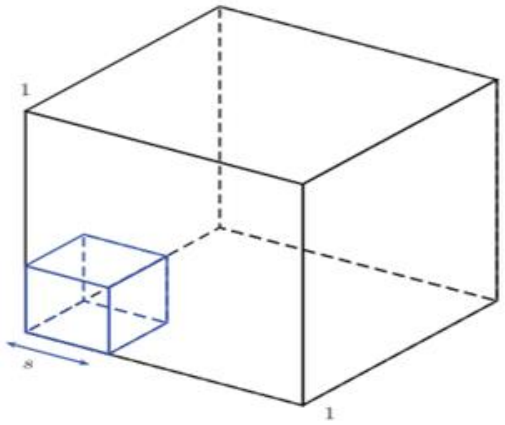
- Changing features and standardizing them has great impact on the loss landscape and optimization
- We can extend this further using a technique called Principal Component Analysis
- In short, PCA will:
  - Rotate mean-centered data
  - Align along the largest orthogonal directions for features before applying standardized scaling
  - Results in more circular contours
  - Simplifies optimization through enabling feature selection – dimension reduction

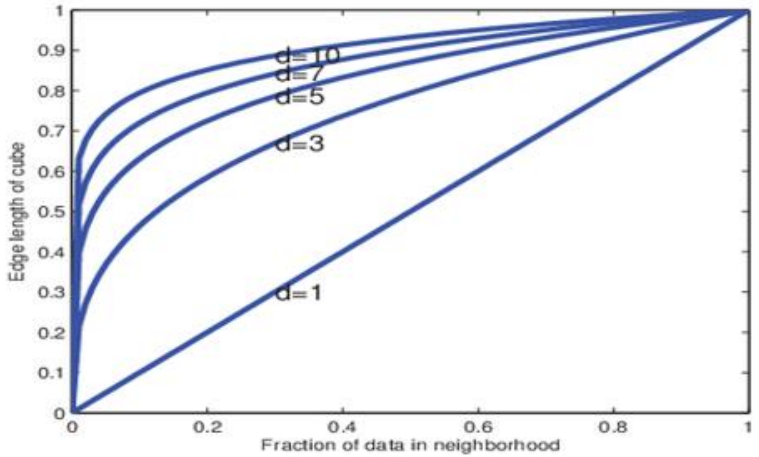
Dimensionality Reduction: Why does it matter?

- Broad Question
  - How can we detect low dimensional structure in high dimensional data
- Motivation
  - Exploratory data analysis: You can easily plot and visualize low dimensional data
  - Compact representation: takes less space
  - Robust statistical modeling: counters the curse of dimensionality

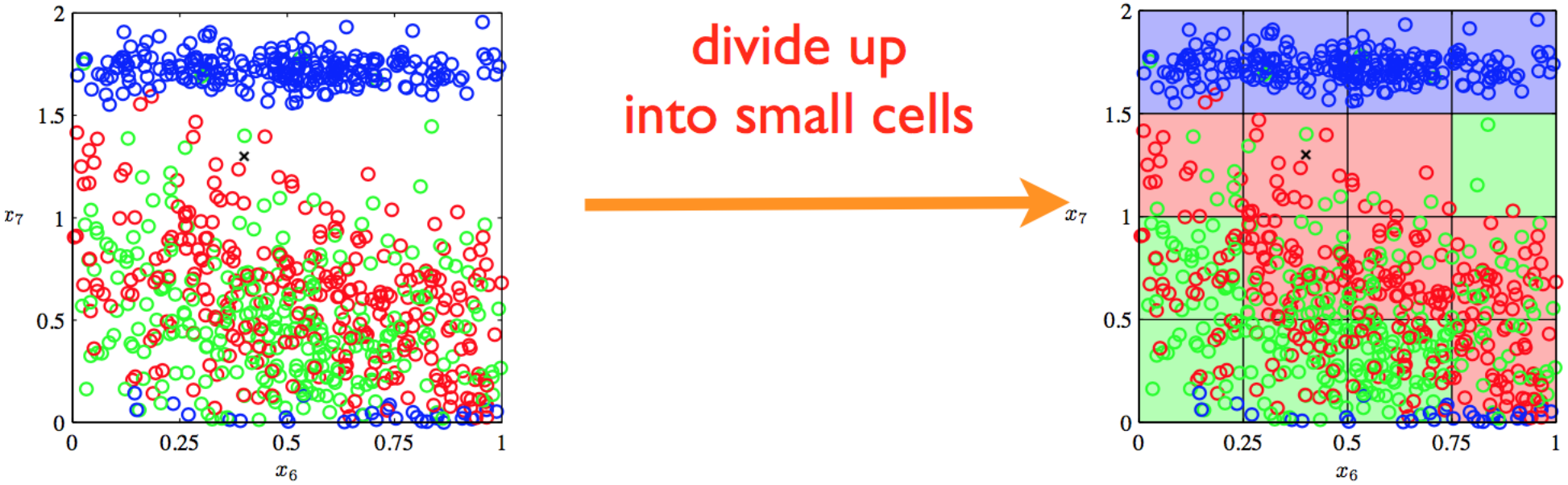
Curse of Dimensionality

- In high dimensional data
  - Intuition tends to fail in higher dimensions about similarity
  - Problems become harder to generalize
  - Harder to systemically search
- On the positive side
  - Blessing of non-uniformity – examples tend not to be uniformly distributed in high dimensions

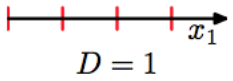


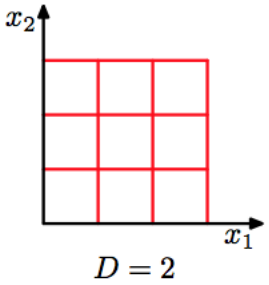


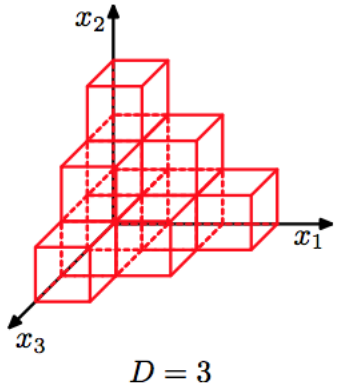
What is the curse of dimensionality: Example with trees



Curse of Dimensionality: Number of Cells to divide







# of cells r^D

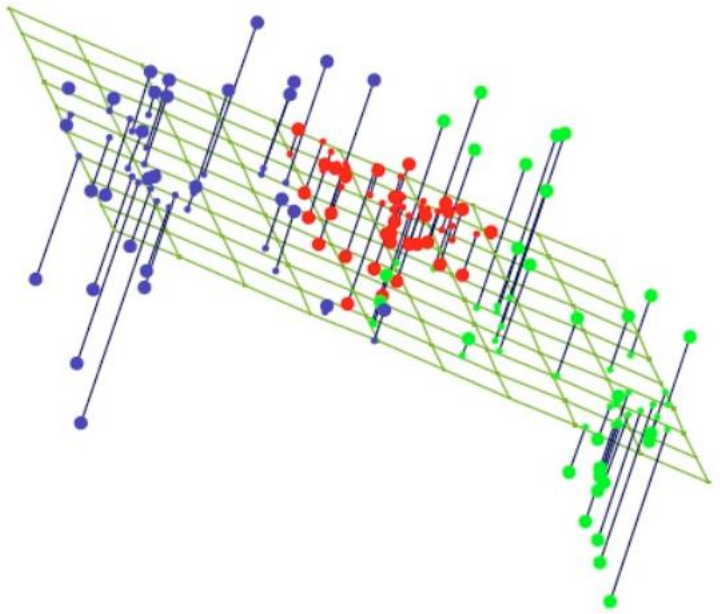
r: number of divisions in each dimension

Large number of cells, even if D is only moderately large
So to cover the whole space reasonably well you need exponentially larger number of training data points

Linear Dimensionality Reduction

To go from X in P dimensional space to Z in M dimensional space where P >> M
Create a linear transformation of

$$z = U^T x$$



Transforming Predictors

- Methods thus far have selected from all predictors x for all dimensions i = 1, … , P
- What if we transform them to z for i = 1, …, M that represent M < P linear combinations of our original P predictors
- That is

$$Z_m = \sum_{j=1}^{P} \phi_{jm} X_j$$

For constants ϕ_{jm}, m = 1, …, M

Fitting Regression

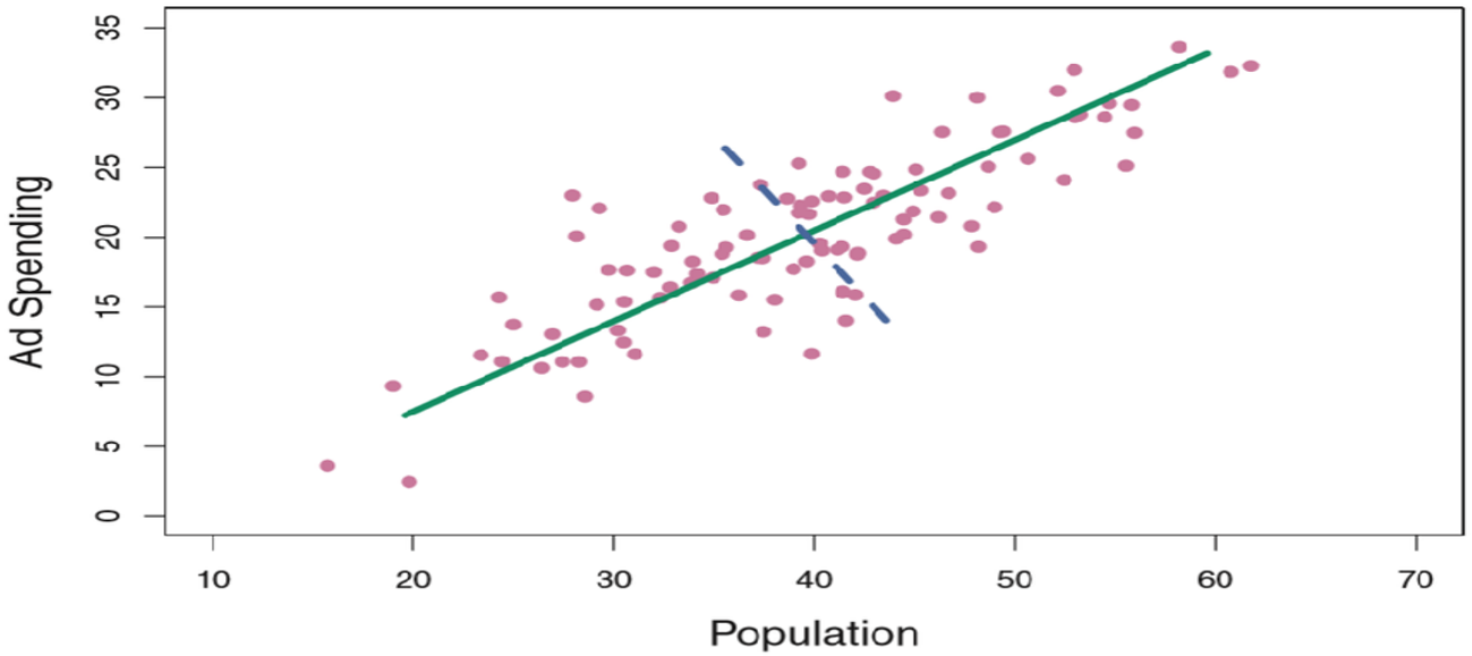
- We can use this to fit

$$y_i = w_0 + \sum_{m=1}^{M} w_m Z_{im} + \epsilon_i$$

For all subjects i from 1 to N.

This results in constants w that are the same linear regression but constrains them in M dimensions instead of P.

Visualizing PCA



PCA: Populations and Ads

- Assume you had a fit regression of the form

$$Z_1 = 0.839 * (pop - \overline{pop}) + 0.544 * (ad - \overline{ad})$$

- We can call 0.839 and 0.544 the principal component loadings – they provide the size and direction of the transformation on each particular axis
- What we want to do is maximize the

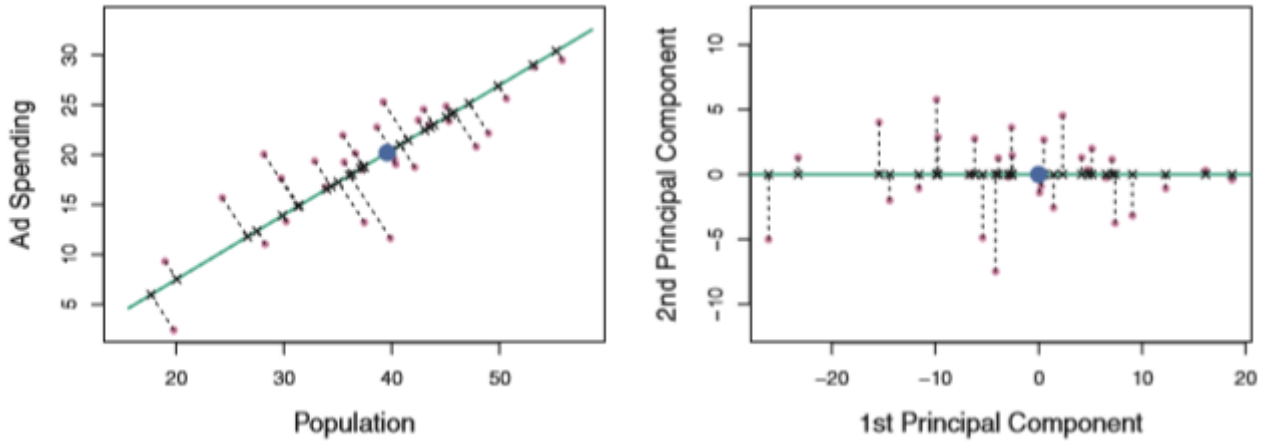
Var $(\phi_1 * (pop - \overline{pop}) + \phi_2 * (ad - \overline{ad})$

So each element has

$$z_{1i} = 0.839 * (pop_i - \overline{pop}) + 0.544 * (ad_i - \overline{ad})$$

And so the z_{1i} and on up to M are the principal component scores

PCA Transformation



PCA Challenges in Unsupervised Learning

- How do you learn these loadings without supervised labels?
- No simple goal to compare against
- Exploratory data analysis means there is no way to check if your answer is correct
- Infeasible to do a bunch of 2D scatter plots across all dimensions p

PCA: Representation

Input: D = $\{x_i\}_{i=1}^{N}, where\ x_i \in \mathbb{R}^p$

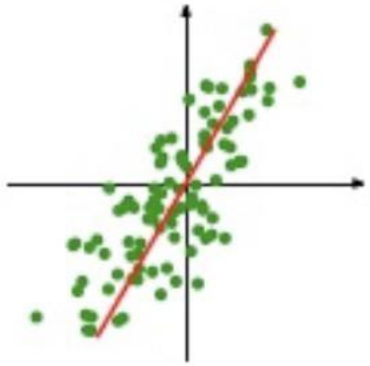
Output: Projected data $\{z_i\}_{i=1}^{N}\ where\ z_i \in \mathbb{R}^M$ and M $\ll$ p

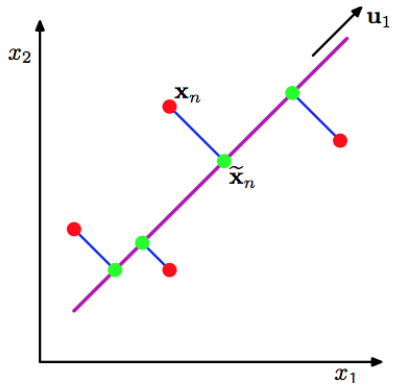
Projection into Subspace: $U \in \mathbb{R}^{pXM}$

$$z_i = U^T x_i$$

$$U^T U = I$$

Evaluation Metric: Many possible metrics can yield the same solution, Maximize the captured variance, minimize the projection error, minimize reconstruction error, etc.





How do we do this: Matrix Diagonalization

- Converting a square matrix into a special type of matrix (i.e. diagonal), which shares the same fundamental properties of an underlying matrix
- Find a square matrix A of dimension D, that can be decomposed into

$$A = P \Lambda P^{-1}$$

- Where

$$\Lambda = diag(\lambda_1, \dots, \lambda_D)$$

The eigenvalues of A

And

$$P = [e_1, \dots, e_D]$$

Where each e is an eigenvector of A

PCA Optimization of an X

- First, create the covariance matrix (which is a square matrix) from X

$$S = \frac{1}{N} X^T X = \frac{1}{N} \sum_{i=1}^{N} x_i x_i^T$$

- Then, diagonalize S (ie compute the eigenvalues and eigenvectors)

$$S = P \, \Lambda \, P^{-1}$$

- Finally, choose the eigenvectors corresponding to some M largest eigenvalues

$$U = [e_1, \dots, e_M] \in \mathbb{R}^{pXM}$$

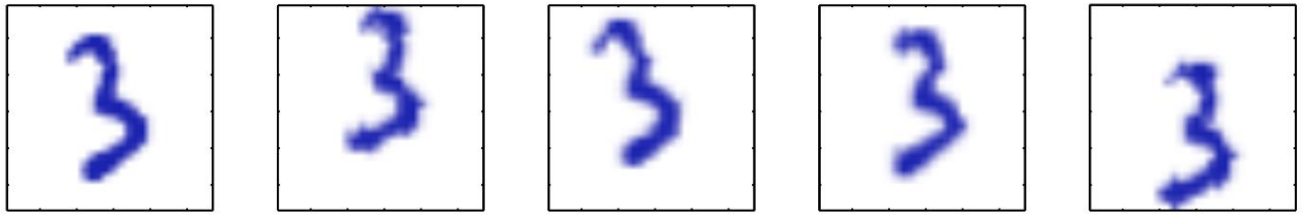
PCA Algorithm

- Step 0: Mean normalize the input features
- Step 1: Compute the covariance matrix S from input matrix X
- Step 2: Diagonalize S and find the eigenvector matrix P
- Step 3: Chose the first M << P eigenvectors or principal components (corresponding to the M largest eigenvalues) and form reduced matrix U
- Step 4: Project data onto the reduced space

$$z_i = U^T x_i$$

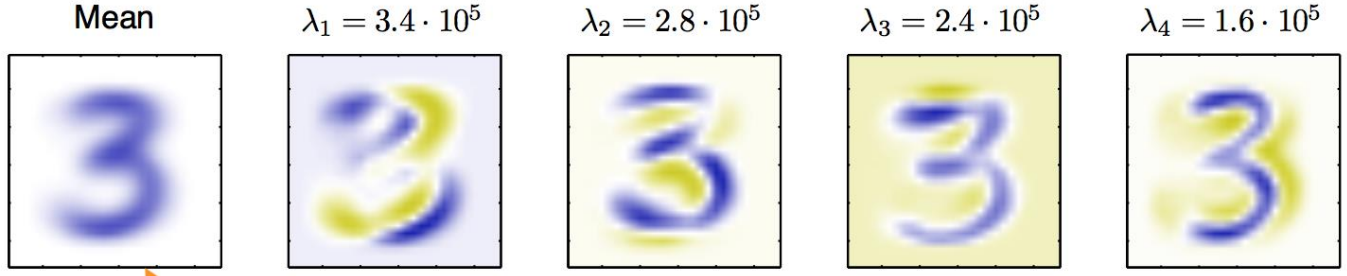
PCA Visualization

Original Images



Eigenvectors

they look like blurred original images



Used to centralize inputs

Applications of PCA

Preprocessing

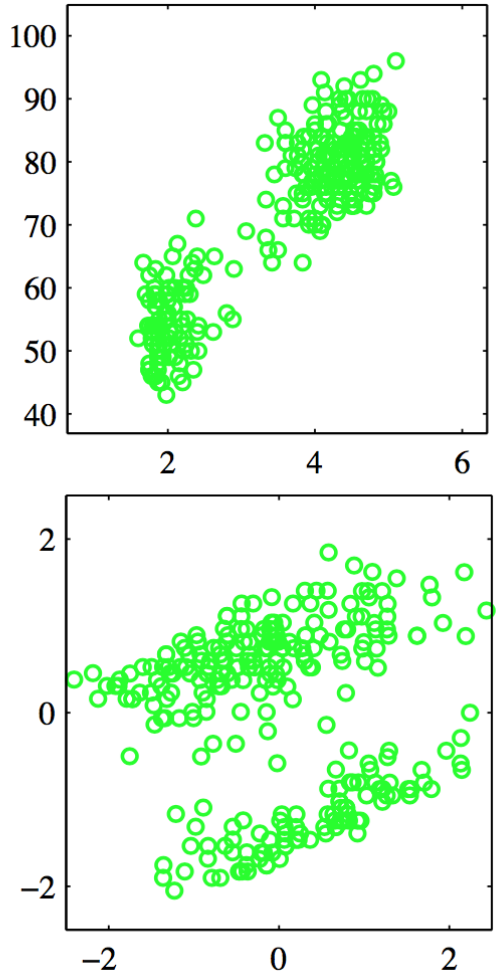
Diagonalize data

$$\boldsymbol{y}_i = \boldsymbol{U}^{\mathrm{T}} \boldsymbol{x}_i$$

Normalize data (whitening)

$$\boldsymbol{y}_i = \boldsymbol{\lambda}^{-1/2} \boldsymbol{U}^{\mathrm{T}} \boldsymbol{x}_i$$

Benefits:
1) depress noisy features
2) couple with other models



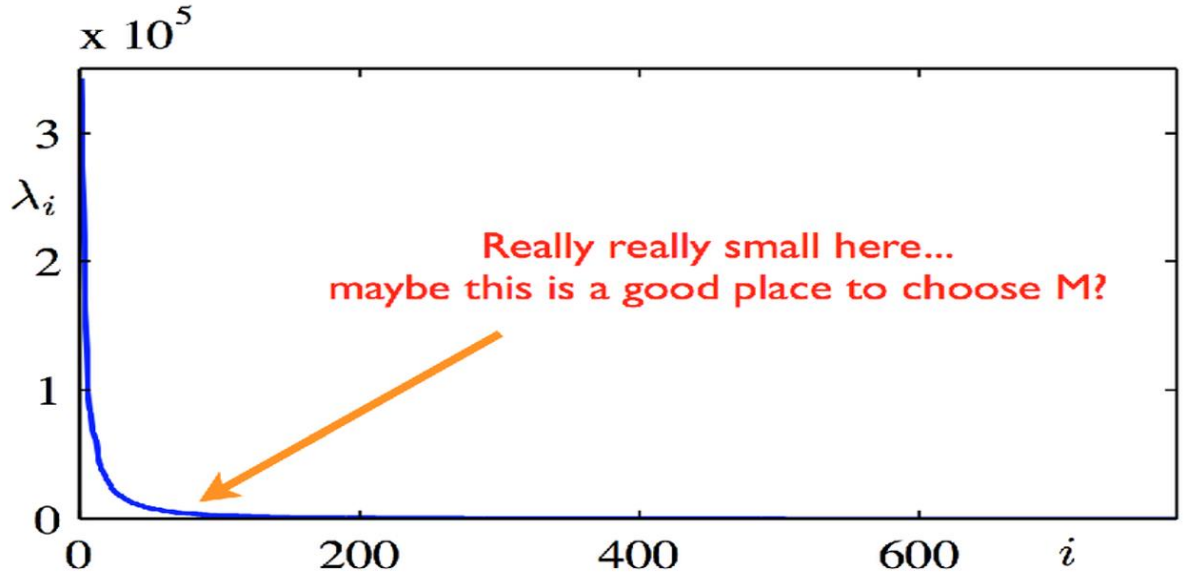
Choosing the right number of components

Plot the eigenspectrum (magnitude of eigenvalues over number of eigenvectors)

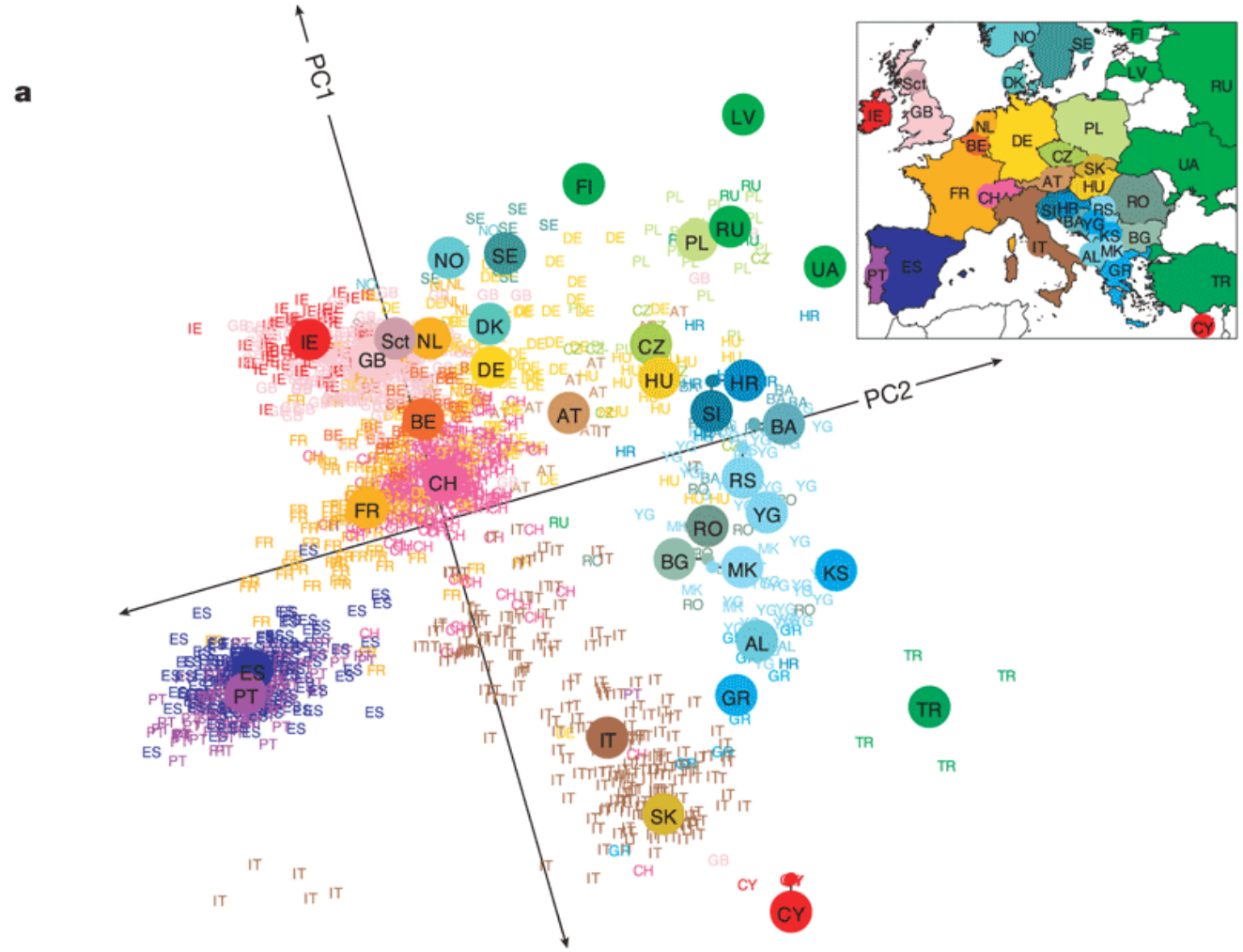
Choose a threshold such as

$$\frac{\sum_{j=1}^{M} \lambda_j}{\sum_{j=1}^{P} \lambda_j} \geq \tau$$

Where it is common to chose 95%, 99% etc.



Applications: Clustering
Finding patterns and structure in unstructured data



Unsupervised learning

- Find patterns/structure/sub-populations in data “knowledge discovery”
- Training data does not contain outputs
- Less well-defined problem with no obvious error metrics
- Examples: topic modeling, market segmentation, handwritten digits, news stories, etc.

K-Means Clustering

- Input D = $\{x_i\}_{i=1}^{N}, where\ x_i \in \mathbb{R}^p$
- Output: Clusters $\mu_1, \dots, \mu_K$
- Decision: Define cluster membership, provide a cluster id assigned to each sample x

$$A(x_i) \in \{1, \dots, K\}$$

- Evaluation Metric: Distortion Measure

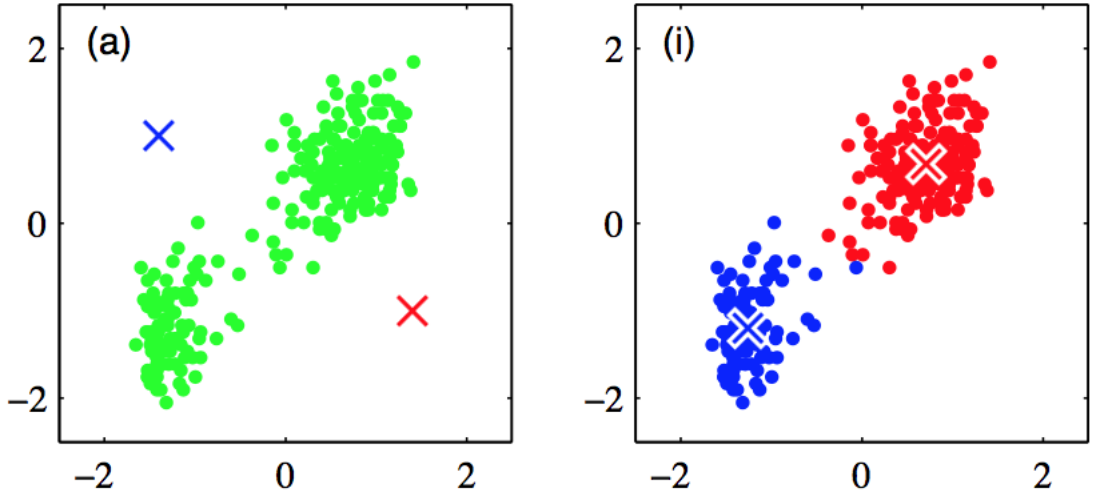
$$J = \sum_{i=1}^{N} \sum_{k=1}^{K} r_{nk} \|x_i - \mu_k\|_2^2$$

Where $r_{nk} = 1$ if $A(x_i) = k$

- Intuition: Data points get assigned to cluster k if they are close to centroid μ_k

K-Means Clustering

- Input D = $\{x_i\}_{i=1}^{N}, where\ x_i \in \mathbb{R}^p$
- Output: Clusters $\mu_1, \ldots, \mu_K$
- Decision: Define cluster membership, provide a cluster id assigned to each sample x
- Evaluation Metric: Distor



Where $r_{nk} = 1$ if $A(x_i) =$

- Intuition: Data points get assigned to cluster k if they are close to centroid μ_k

K – means Algorithm

- Optimization Function

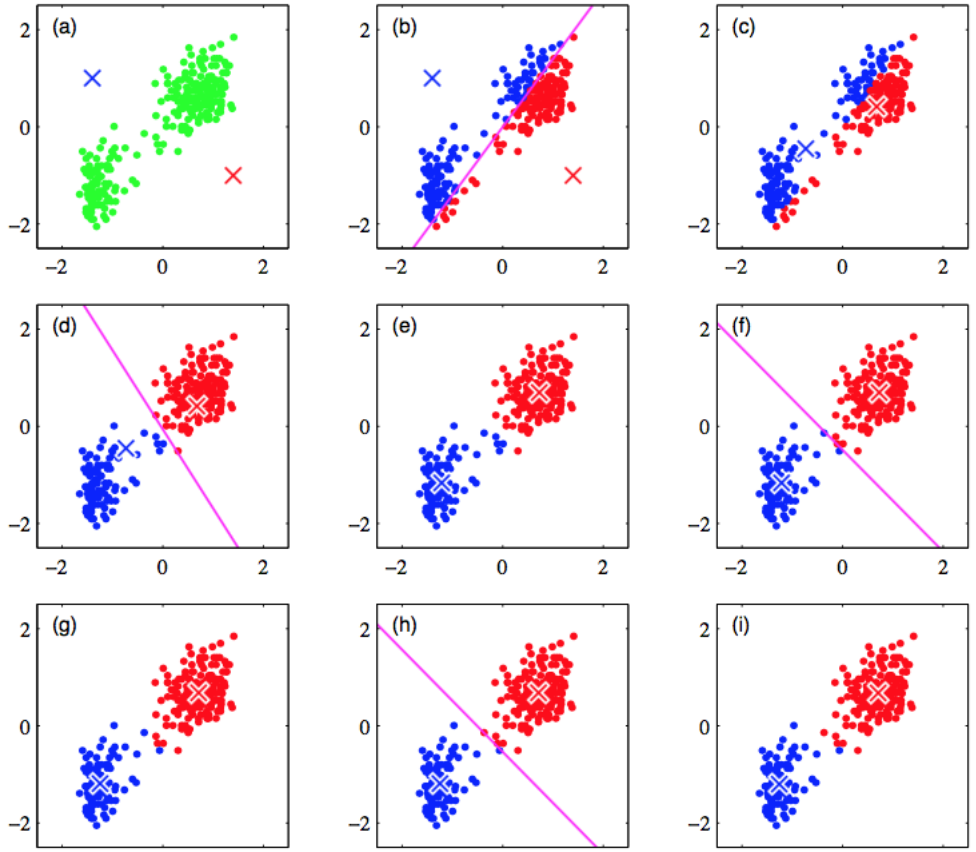
$$\min_{r_{nk}} J = \min_{r_{nk}} \sum_{i=1}^{N} \sum_{k=1}^{K} r_{nk} \|x_i - \mu_k\|_2^2$$

- Step 0: Initialize μ_k to some random values
- Step 1: Assume the current μ_k is fixed, minimize J over r_{nk} which leads to cluster assignment
- Step 2: Assume the fixed cluster assignment, update the cluster centroids as in

$$\mu_k = \frac{\sum r_{nk}\, x_n}{\sum r_{nk}}$$

- Step 3: decide to stop or return to step 1

Visualization of K-Means



Best Performance: PCA and Then Cluster

- PCA! Know how to use libraries to reduce dimensions
- K-Means – know how to determine if there is underlying structure in you rdata
- Next time: Midterm 1 is Tuesday, March 21