Machine Learning

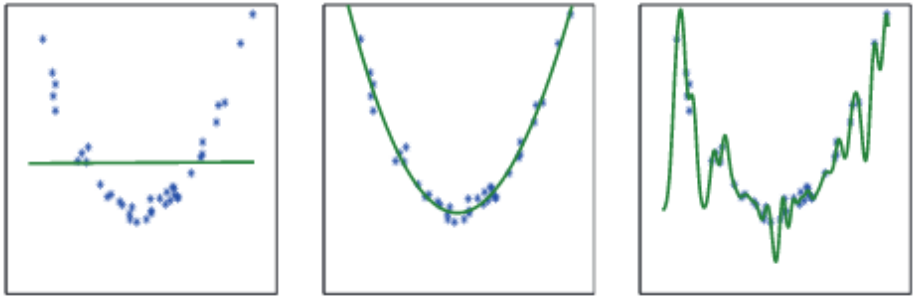
Clustering

Jeff Abrahamson

août 2019

Review and Concepts

Underfitting, overfitting



Random Forest

scikit-learn behaviour:

- Sample size is full training set.
- If `bootstrap=true` then sample with replacement.
- If $n = n'$, expect $1 - 1/e \approx 63.2\%$ repeats.

PCA

Principle component analysis

Analyse en composantes principales

Motivation

Remember the Curse of Dimensionality?

Principle

- Linear transformations have axes
- Find them (eigenvectors of the covariance matrix)
- Pick the biggest ones

Principle

- Linear transformations have axes
- Find them (eigenvectors of the covariance matrix)
- Pick the biggest ones

Fitting an n-dimensional ellipsoid to the data

Uses

- Exploratory data analysis
- Compression
- Visualisation

Also known as

- Discrete Kosambi-KarhunenLoève transform (KLT) (signal processing)
- Hotelling transform (multivariate quality control)
- Proper orthogonal decomposition (POD) (ME)
- Singular value decomposition (SVD), Eigenvalue decomposition (EVD) (linear algebra)
- Etc.

History

- Invented by Karl Pearson in 1901
- Invented (again) and named by Harold Hotelling in 1930's
- Also known as. . .

History

- Invented by Karl Pearson in 1901
- Invented (again) and named by Harold Hotelling in 1930's
- Also known as...

It's a long list, every field uses a different name.

Face Recognition

Eigenfaces

- Sirovich and Kirby (1987)
- Turk and Pentland (1991)

Turk, Matthew A and Pentland, Alex P. Face recognition using eigenfaces. Computer Vision and Pattern Recognition, 1991. Proceedings CVPR'91., IEEE Computer Society Conference on 1991.

Eigenfaces

Want: a low-dimensional representation of a face

Plan: cluster simplified faces

Eigenfaces

Viewed as compression:

- Use PCA on face images to form a set of basis features
- Use eigenpictures to reconstruct original faces

Eigenfaces

Eigenfaces algorithm

Let $X = \{x_1, x_2, \ldots, x_n\}$ be a random vector with observations $x_i \in \mathbb{R}^d$.

Compute

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

OpenCV

Eigenfaces algorithm

Compute the covariance matrix S:

$$\begin{aligned} S_{i,j} &= \mathbf{Cov}(x_i, x_j) \\ &= \mathbf{E}[(x_i - \mu_i)(x_j - \mu_j)^T] \end{aligned}$$

$$S = (S_{i,j})$$

Eigenfaces algorithm

Compute the eigenvectors of S:

$$Sv_i = \lambda_i v_i \qquad i = 1, 2, \ldots, n$$

Sort the eigenvectors in decreasing order.

We want the k principal components, so take the first k.

Eigenfaces algorithm

Compute the eigenvectors of S:

$$Sv_i = \lambda_i v_i \qquad i = 1, 2, \ldots, n$$

Sort the eigenvectors in decreasing order.

We want the k principal components, so take the first k.

This is PCA.

Eigenfaces algorithm

The k principal components of the observed vector x are then given by

$$y = W^T(x - \mu)$$

where

$$W = \begin{bmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_k \\ | & | & & | \end{bmatrix}$$

Eigenfaces algorithm

The reconstruction from the PCA basis is then

$$x = Wy + \mu$$

Eigenfaces algorithm

So the plan is this:

- Project all training samples in the PCA subspace
- Project the query into the PCA subspace
- Find the nearest neighbour to the projected query image among the projected training images

Eigenfaces algorithm

Eigenfaces algorithm

Some advantages:

- Easy, relatively inexpensive
- Recognition cheaper than preprocessing
- Reasonably large database possible

Eigenfaces algorithm

Some problems:

- Need controlled environment
- Needs straight-on view
- Sensitive to expression changes
- If lots of variance is external (e.g., lighting)...

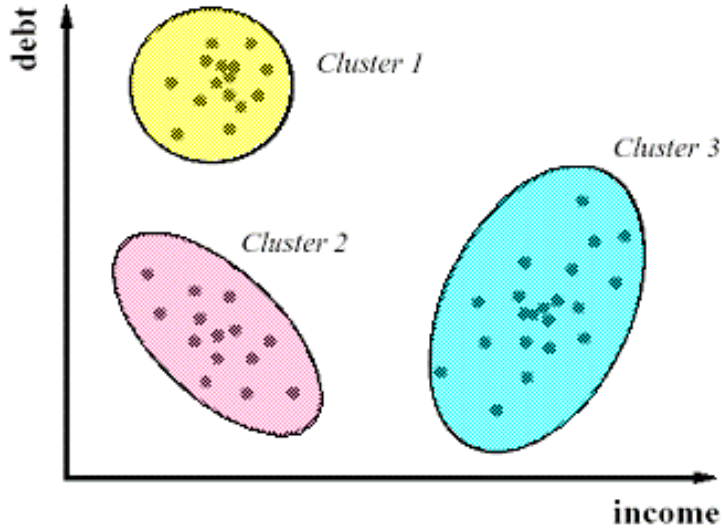
Clustering

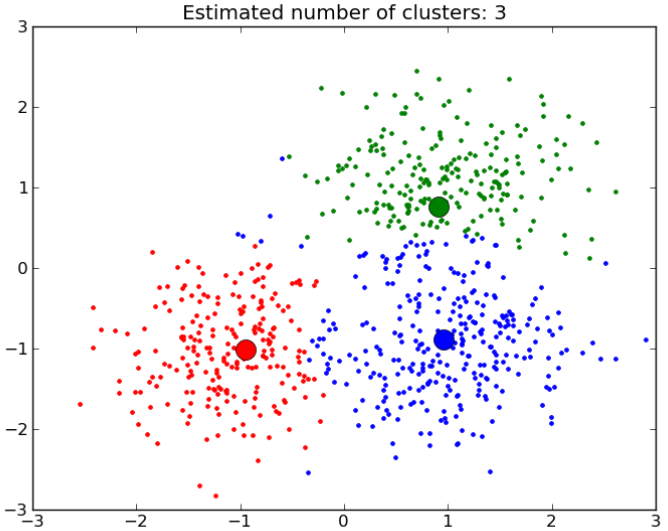
The Problem

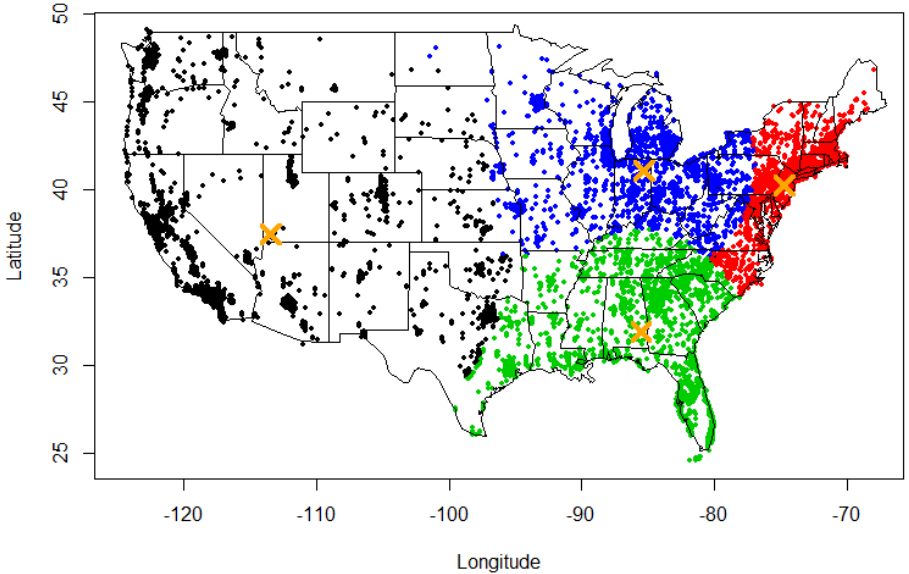
Have points $d = \{d_1, \ldots, d_n\}$.

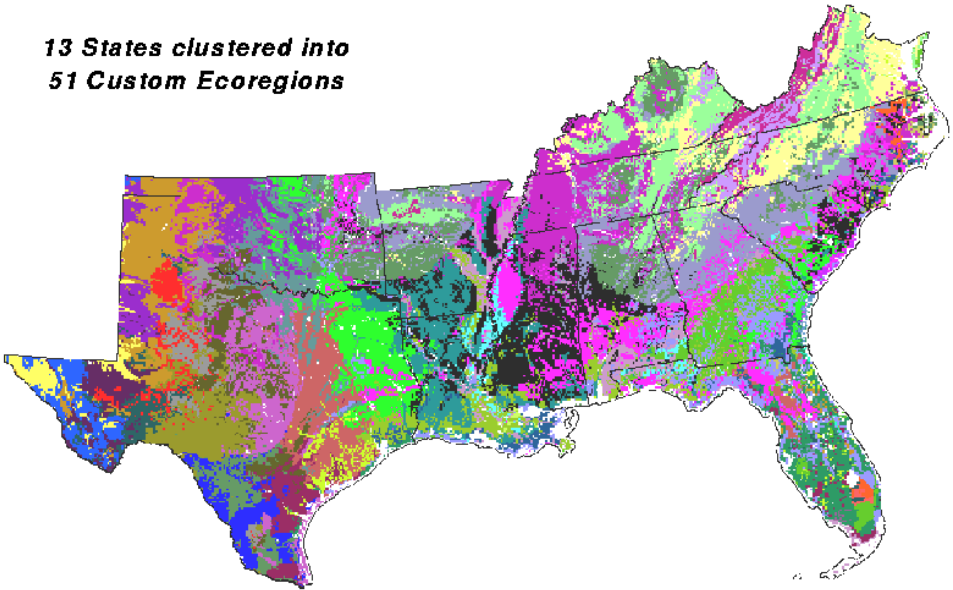
Have number of clusters k.

Want: an assignment of points to clusters









The Algorithm

1. Assign points to clusters at random
2. Repeat until stable:
    1. Compute centroids of each cluster
    2. Assign points to nearest centroid

Cost function

$$\text{cost} = \sum_i \sum_j |x_j - \mu_i|$$

Silhouette coefficient

Points $d = \{d_1, \ldots, d_n\}$

Clusters $K = \{c_1, \ldots, c_k\}$.

Cluster c_{d_i} is the centroid of d_i.

Silhouette coefficient

Points $d = \{d_1, \ldots, d_n\}$

Clusters $K = \{c_1, \ldots, c_k\}$.

Cluster c_{d_i} is the centroid of d_i.

Let a_i be the average dissimilarity of d_i to all points in its cluster.

Let b_i be the least average dissimilarity of d_i to any cluster other than k_{d_i}

Silhouette coefficient

$$s_i = \frac{b_i - a_i}{\max\{a_i, b_i\}}$$

Silhouette coefficient

$$s_i = \frac{b_i - a_i}{\max\{a_i, b_i\}}$$

$$s_i = \begin{cases} 1 - a_i/b_i & \text{if } a_i < b_i \\ 0 & \text{if } a_i = b_i \\ b_i/a_i - 1 & \text{if } a_i > b_i \end{cases}$$

Silhouette coefficient

$$s_i = \frac{b_i - a_i}{\max\{a_i, b_i\}}$$

$$s_i = \begin{cases} 1 - a_i/b_i & \text{if } a_i < b_i \\ 0 & \text{if } a_i = b_i \\ b_i/a_i - 1 & \text{if } a_i > b_i \end{cases}$$

So $s_i \in [-1, 1]$

Silhouette coefficient

s_i near 1 $\iff$ d_i well clustered

s_i near 0 $\iff$ d_i on the border between two clusters

s_i near -1 $\iff$ d_i poorly clustered

Silhouette coefficient

Consider $\overline{s_i}$ over $i \in c_j$ for cluster c_j

Silhouette coefficient

Consider $\overline{s_i}$

video time

Anomaly Detection

Introduction to Anomaly Detection

- Supervised
- Unsupervised

Introduction to Anomaly Detection

Supervised anomaly detection:

- Training data: normal, abnormal
- Train a classifier

So reduced to existing problem of supervised classification.

Introduction to Anomaly Detection

Unsupervised anomaly detection:

- Mostly, this is clustering
- Increasingly, this is neural networks in advanced applications

Introduction to Anomaly Detection

Applications:

- Intrusion detection (physical or electronic)
- Fraud detection
- Health monitoring (people, animals, machines)

Introduction to Anomaly Detection

Techniques:

- Density: kNN, local outlier factor
- SVM
- Clustering: *k*-Means

kNN techniques and variations

- Voronoi diagrams
- aNN

LOF

- Measure average density using kNN
- Points with low local density are suspect outliers
- There is no good thresholding technique

k-Means

Examples

ping times

Examples

httpd response times

Examples

single/multiple host access abuse (DOS/DDOS)

Examples

bank card fraud

Examples

spam