Lecture Notes for

Machine Learning in Python

[👨‍🏫, 👨‍💻, 🐍, 👨‍🔬]

Professor Eric Larson

Visualization

Class Logistics and Agenda

- Finish Visualization Demo
- Town Hall
- Next Time:
  - Dimensionality Reduction
    - PCA
    - Sampling
    - Kernel Methods
  - Images

Class Overview, by topic

Table Data Visualization
Numpy, Pandas, Seaborn
Overviews with some in-depth discussion

Dimension Reduction and Image Processing
Scikit-learn, Scikit Image,
Intuition only, Some mathematics

Linear and Logistic Regression
Numpy, Recreate API for Scikit-learn
Detailed mathematics for simple optimization
intuition for advanced optimization

Neural Networks and Back Prop.
Numpy
Detailed mathematics for NN operations

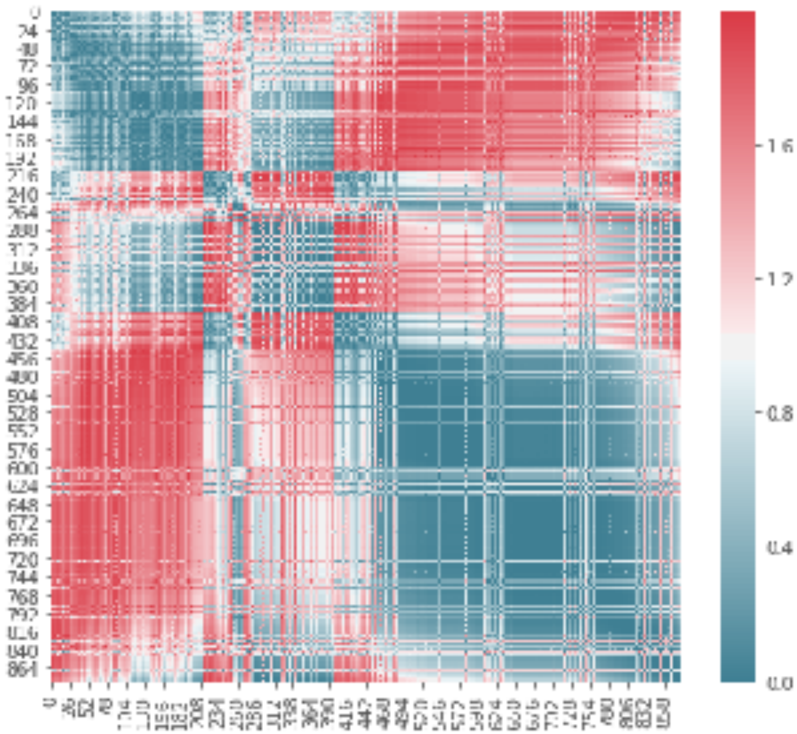
Wide and Deep Networks | **Convolutional Networks** | **Recurrent Networks**
Keras, Tensorflow
Intuition, Detailed implement.

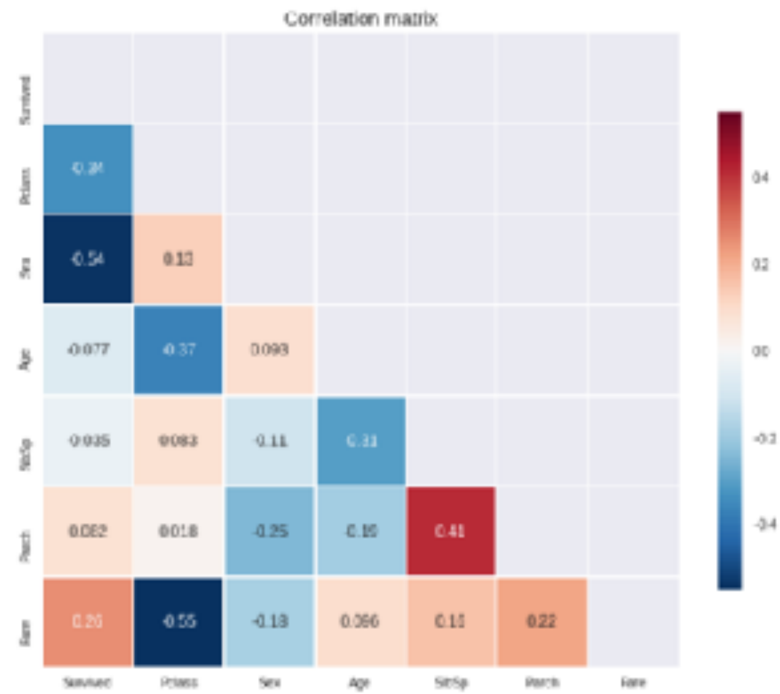
Ethics in Language Models

ConceptNet
Case studies

What is the difference in these plots?

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Embarked	2	3	male	Q	S
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	S	0	1	1	0	1
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.2833	C	0	0	0	0	0
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	S	0	1	0	0	1





Let’s look at some graphs

Demo

- You tell me what conclusions we are getting from these graphs
    - Histogram
    - KDE
    - HeatMaps and Correlation
    - Scatter and Scatter Matrix
    - Box / Violin / Swarm

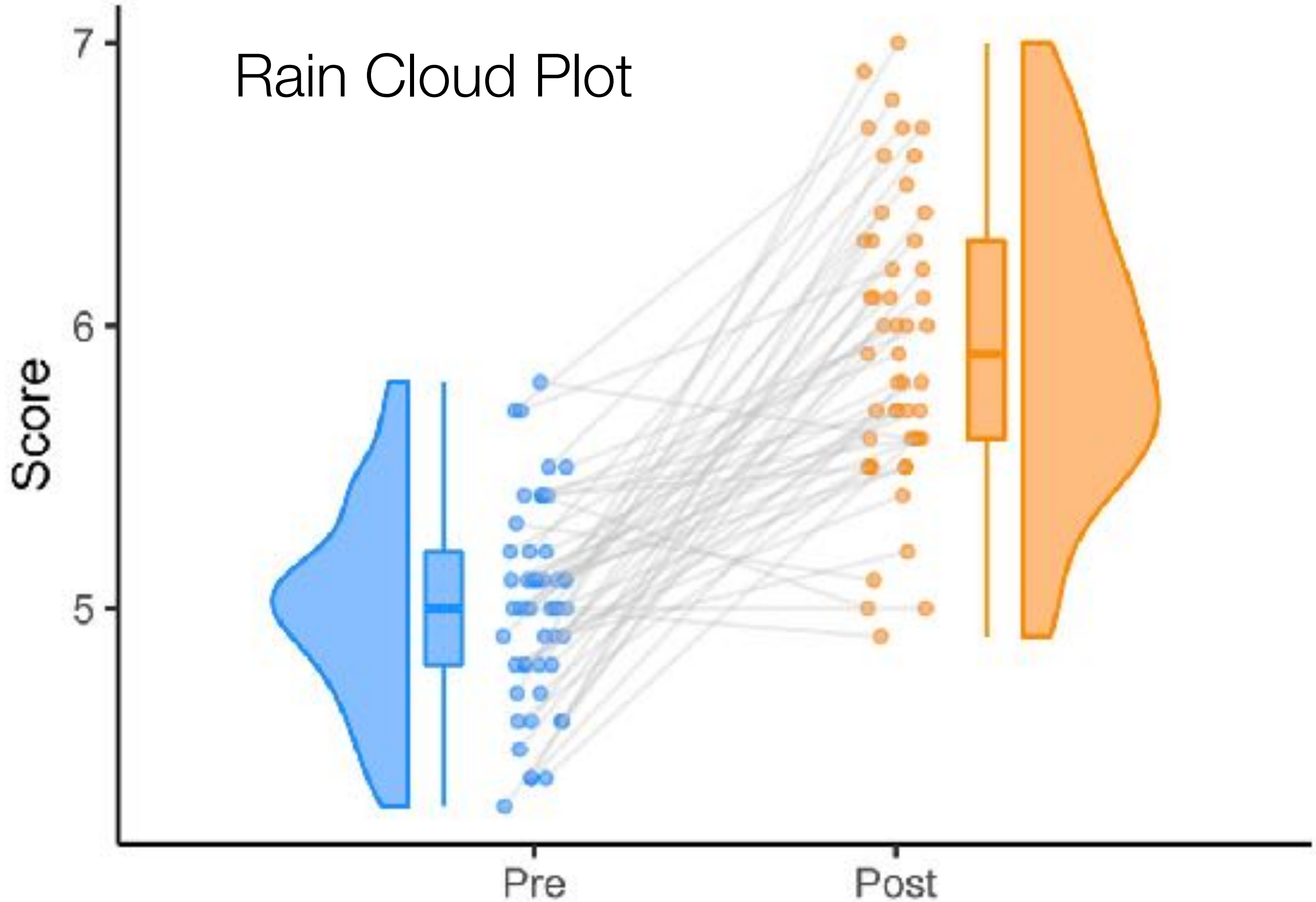
`03.Data Visualization.ipynb`

Matplotlib

Seaborn

Plotly

Now you have visualization building blocks



Understanding **Before** Lecture Demo

Understanding **After** Lecture Demo

Lab One: Town Hall

Supplemental Slides

Visualization Techniques: Contour Plots

- Contour plots
  - Useful when a continuous attribute is measured on a spatial grid
  - They partition the plane into regions of similar values
  - The contour lines that form the boundaries of these regions connect points with equal values
  - The most common example is contour maps of elevation
  - Can also display temperature, rainfall, air pressure, etc.
    - An example for Sea Surface Temperature (SST) is provided on the next slide

Other Visualization Techniques

- Star Plots
    - Similar approach to parallel coordinates, but axes radiate from a central point
    - The line connecting the values of an object is a polygon
- Chernoff Faces
    - Approach created by Herman Chernoff
    - This approach associates each attribute with a characteristic of a face
    - The values of each attribute determine the appearance of the corresponding facial characteristic
    - Each object becomes a separate face
    - Relies on human's ability to distinguish faces

Challenges of Data Mining

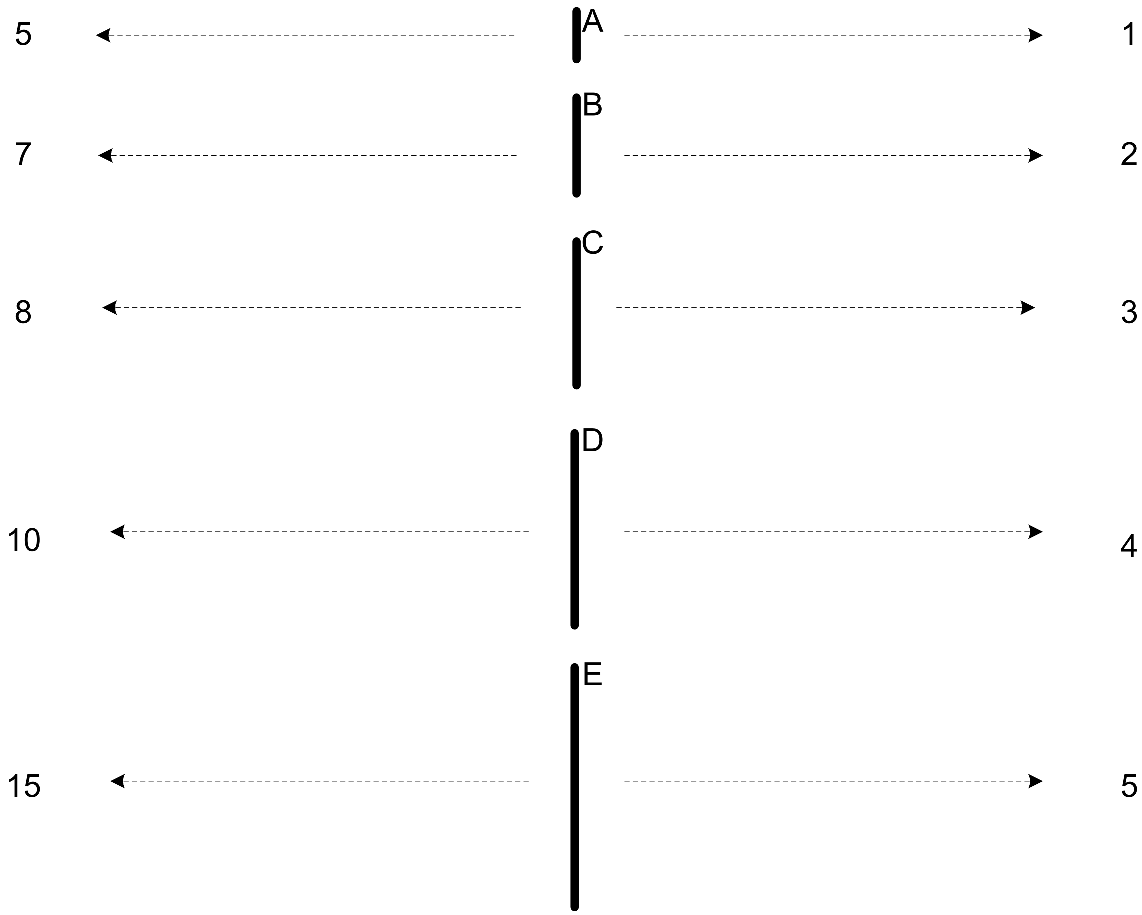
- Scalability
- Dimensionality
- Complex and Heterogeneous Data
- Data Quality
- Data Ownership and Distribution
- Privacy Preservation
- Streaming Data

Important Characteristics of Structured Data

- Dimensionality
  - Curse of Dimensionality
- Sparsity
  - Only presence counts
- Resolution
  - Patterns depend on the scale

Measurement of Length

- The way you measure an attribute is somewhat may not match the attributes properties.



Sampling

- **Sampling is the main technique employed for data selection.**
  - **It is often used for both the preliminary investigation of the data and the final data analysis.**

- **Statisticians sample because obtaining the entire set of data of interest is too expensive or time consuming.**

- **Sampling is used in data mining because processing the entire set of data of interest is too expensive or time consuming.**

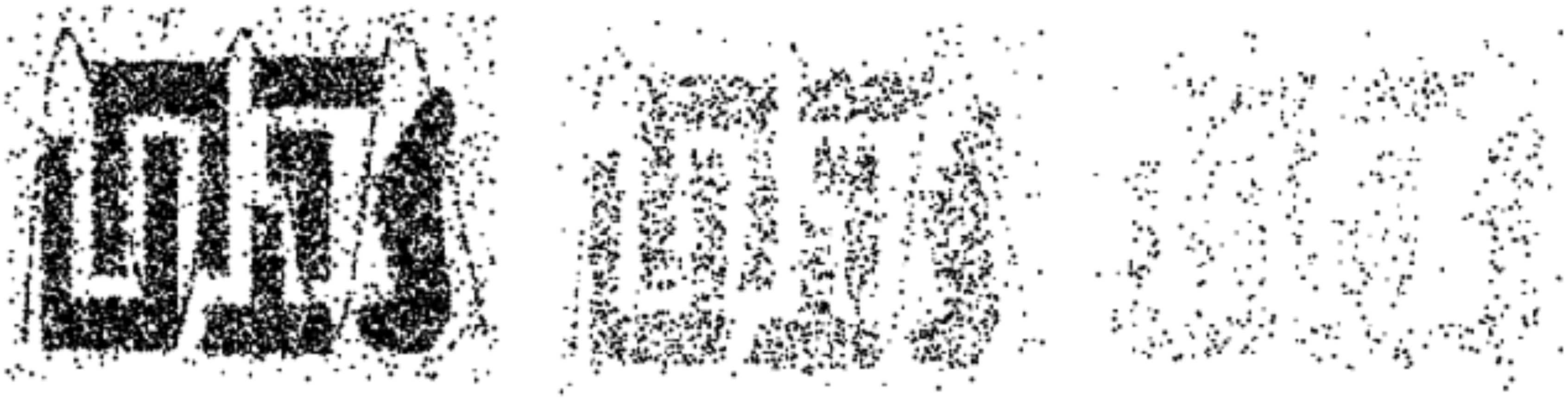
Sampling …

- The key principle for effective sampling is the following:
  - using a sample will work almost as well as using the entire data sets, if the sample is representative
  - A sample is representative if it has approximately the same property (of interest) as the original set of data

Types of Sampling

- Simple Random Sampling
    - There is an equal probability of selecting any particular item
- Sampling without replacement
    - As each item is selected, it is removed from the population
- Sampling with replacement
    - Objects are not removed from the population as they are selected for the sample.
        - In sampling with replacement, the same object can be picked up more than once
- Stratified sampling
    - Split the data into several partitions; then draw random samples from each partition

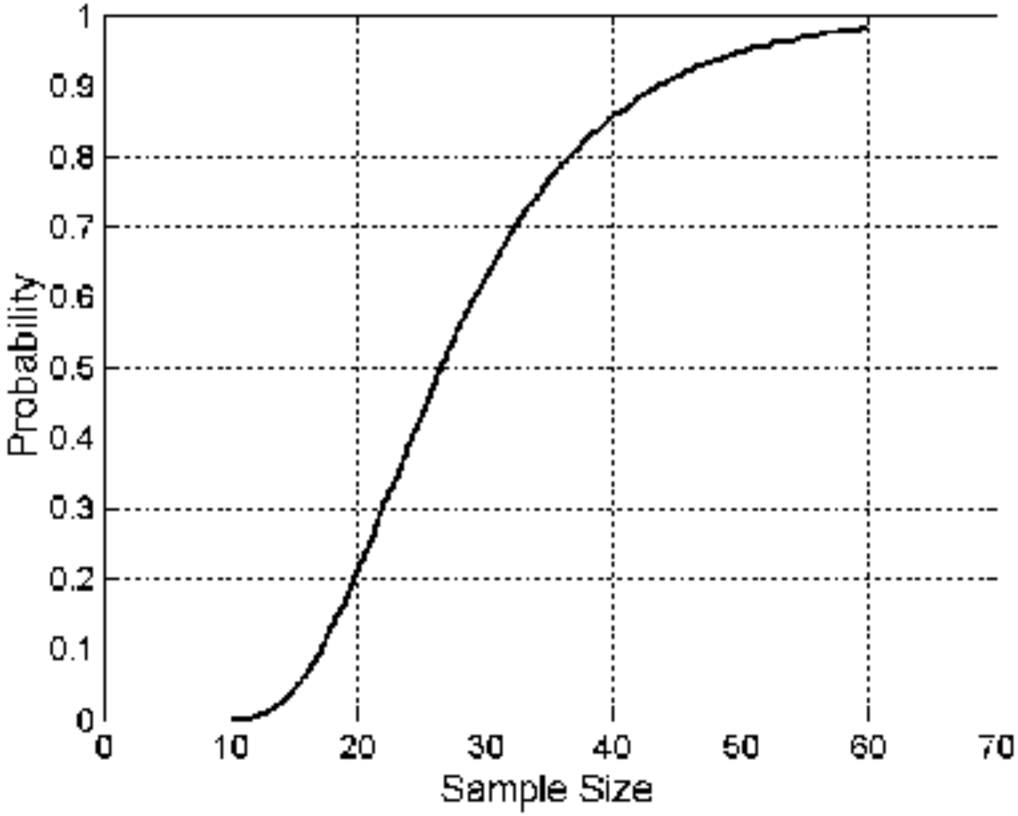
Sample Size



8000 points　　2000 Points　　500 Points

Sample Size

- **What sample size is necessary to get at least one object from each of 10 groups.**



Similarity and Dissimilarity

- Similarity
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- Dissimilarity
  - Numerical measure of how different are two data objects
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- Proximity refers to a similarity or dissimilarity

Similarity/Dissimilarity for Simple Attributes

p and *q* are the attribute values for two data objects.

Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p \neq q \end{cases}$	$s = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$
Ordinal	$d = \frac{\lvert p-q \rvert}{n-1}$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - \frac{\lvert p-q \rvert}{n-1}$
Interval or Ratio	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{1+d}$ or $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Table 5.1. Similarity and dissimilarity for simple attributes

Euclidean Distance

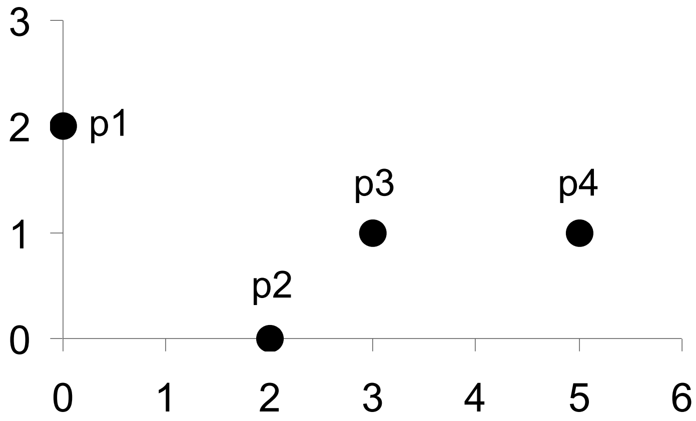
- Euclidean Distance

$$dist = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

Where n is the number of dimensions (attributes) and p_k and q_k are, respectively, the k^{th} attributes (components) or data objects p and q.

- Standardization is necessary, if scales differ.

Euclidean Distance



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance Matrix

Minkowski Distance

- Minkowski Distance is a generalization of Euclidean Distance

$$dist = \left(\sum_{k=1}^{n} | p_k - q_k |^r \right)^{\frac{1}{r}}$$

Where r is a parameter, n is the number of dimensions (attributes) and p_k and q_k are, respectively, the kth attributes (components) or data objects p and q.

Minkowski Distance: Examples

- $r = 1$. City block (Manhattan, taxicab, L_1 norm) distance.
  - A common example of this is the Hamming distance, which is just the number of bits that are different between two binary vectors
- $r = 2$. Euclidean distance
- $r \rightarrow \infty$. "supremum" (L_{max} norm, L_{∞} norm) distance.
  - This is the maximum difference between any component of the vectors
- Do not confuse *r* with *n*, i.e., all these distances are defined for all numbers of dimensions.

Minkowski Distance

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

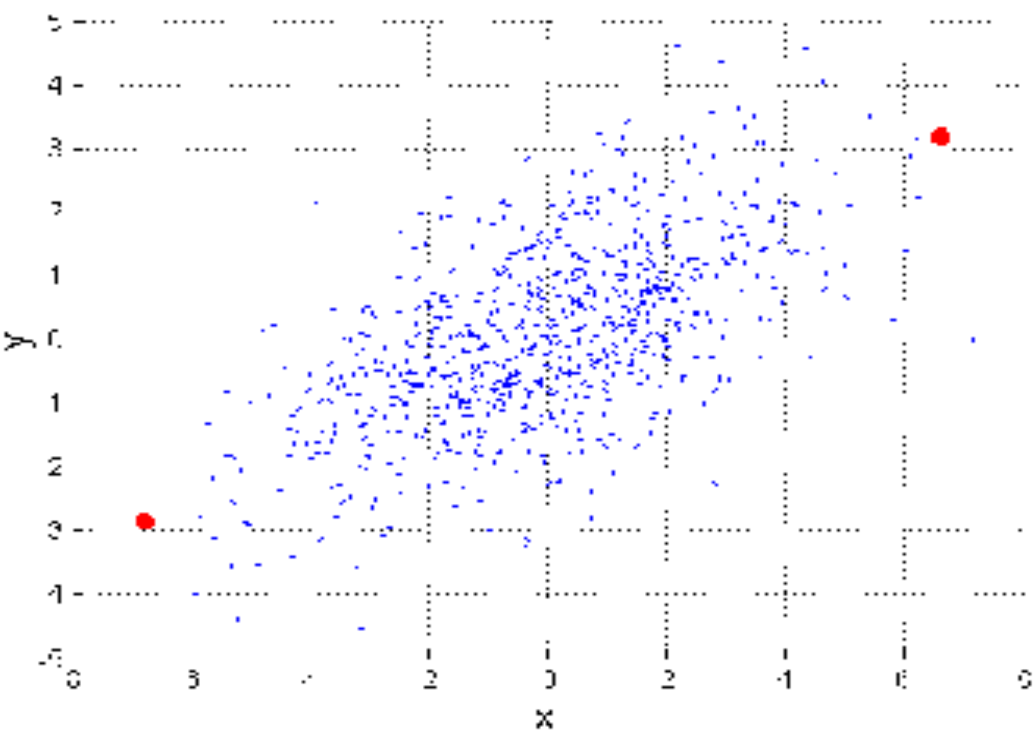
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

L_∞	p1	p2	p3	p4
p1	0	2	3	5
p2	2	0	1	3
p3	3	1	0	2
p4	5	3	2	0

Distance Matrix

Mahalanobis Distance

$$mahalanobis(p,q) = (p-q)\sum^{-1}(p-q)^T$$

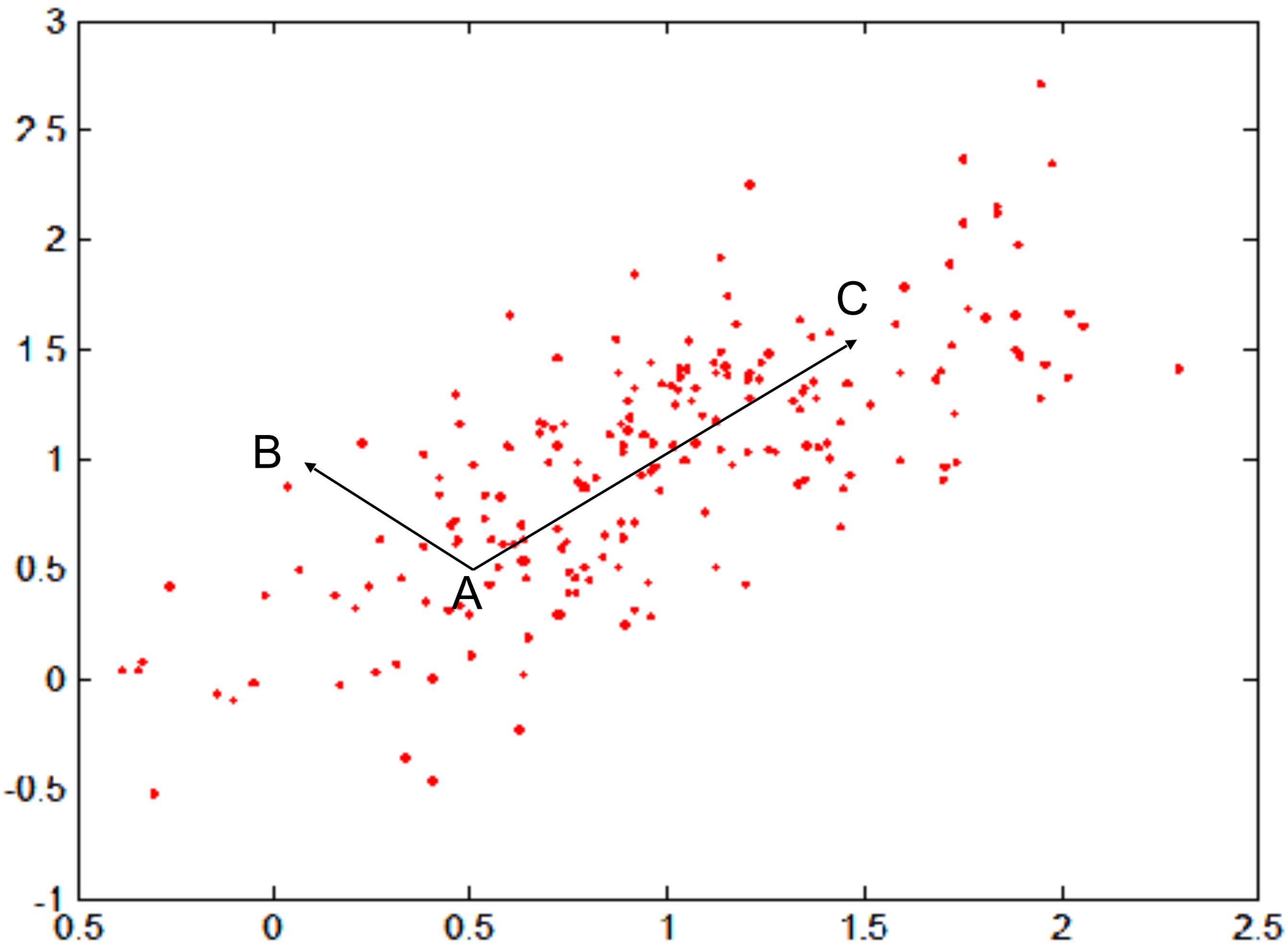


Σ is the covariance matrix of the input data X

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij}-\overline{X}_j)(X_{ik}-\overline{X}_k)$$

For red points, the Euclidean distance is 14.7, Mahalanobis distance is 6.

Mahalanobis Distance



Covariance Matrix:

$$\Sigma = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix}$$

A: (0.5, 0.5)

B: (0, 1)

C: (1.5, 1.5)

Mahal(A,B) = 5

Mahal(A,C) = 4

Common Properties of a Distance

- Distances, such as the Euclidean distance, have some well known properties.

  1. $d(p, q) \geq 0$ for all p and q and $d(p, q) = 0$ only if $p = q$. (Positive definiteness)
  i. $d(p, q) = d(q, p)$ for all p and q. (Symmetry)
  1. $d(p, r) \leq d(p, q) + d(q, r)$ for all points p, q, and r. (Triangle Inequality)

  where $d(p, q)$ is the distance (dissimilarity) between points (data objects), p and q.

1. A distance that satisfies these properties is a metric

Common Properties of a Similarity

- Similarities, also have some well known properties.

1. $s(p, q) = 1$ (or maximum similarity) only if $p = q$.
2. $s(p, q) = s(q, p)$ for all p and q. (Symmetry)

where $s(p, q)$ is the similarity between points (data objects), p and q.

Similarity Between Binary Vectors

- Common situation is that objects, *p* and *q*, have only binary attributes

- Compute similarities using the following quantities
  M_{01} = the number of attributes where p was 0 and q was 1
  M_{10} = the number of attributes where p was 1 and q was 0
  M_{00} = the number of attributes where p was 0 and q was 0
  M_{11} = the number of attributes where p was 1 and q was 1

- Simple Matching and Jaccard Coefficients
  SMC = number of matches / number of attributes
  $= (M_{11} + M_{00}) / (M_{01} + M_{10} + M_{11} + M_{00})$

  J = number of 11 matches / number of not-both-zero attributes values
  $= (M_{11}) / (M_{01} + M_{10} + M_{11})$

SMC versus Jaccard: Example

$p =$ 1 0 0 0 0 0 0 0 0 0

$q =$ 0 0 0 0 0 0 1 0 0 1

$M_{01} = 2$ (the number of attributes where p was 0 and q was 1)

$M_{10} = 1$ (the number of attributes where p was 1 and q was 0)

$M_{00} = 7$ (the number of attributes where p was 0 and q was 0)

$M_{11} = 0$ (the number of attributes where p was 1 and q was 1)

$$SMC = (M_{11} + M_{00})/(M_{01} + M_{10} + M_{11} + M_{00}) = (0+7) / (2+1+0+7) = 0.7$$

$$J = (M_{11}) / (M_{01} + M_{10} + M_{11}) = 0 / (2 + 1 + 0) = 0$$

Cosine Similarity

- If d_1 and d_2 are two document vectors, then

$$\cos(d_1, d_2) = (d_1 \bullet d_2) / ||d_1|| \, ||d_2|| ,$$

where $\bullet$ indicates vector dot product and $|| d ||$ is the length of vector d.

- Example:

$$d_1 = 3\ 2\ 0\ 5\ 0\ 0\ 0\ 2\ 0\ 0$$
$$d_2 = 1\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 2$$

$$d_1 \bullet d_2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$$

$$||d_1|| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$$

$$||d_2|| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.245$$

$$\cos(d_1, d_2) = .3150$$

Extended Jaccard Coefficient (Tanimoto)

- Variation of Jaccard for continuous or count attributes
  - Reduces to Jaccard for binary attributes

$$T(p,q) = \frac{p \bullet q}{|p\|^2 + \|q\|^2 - p \bullet q}$$

Correlation

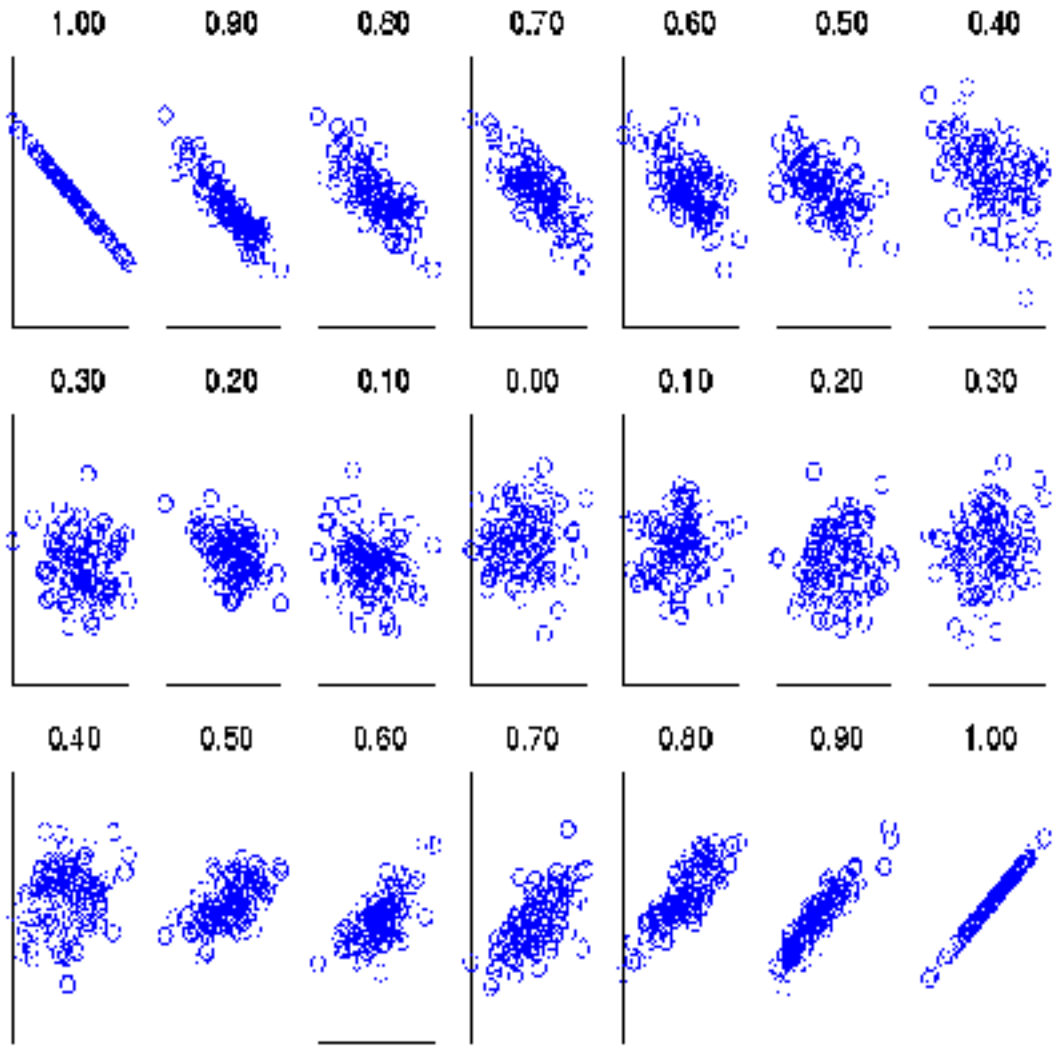
- Correlation measures the linear relationship between objects
- To compute correlation, we standardize data objects, p and q, and then take their dot product

$$p'_k = (p_k - mean(p)) / std(p)$$

$$q'_k = (q_k - mean(q)) / std(q)$$

$$correlation(p, q) = p' \bullet q'$$

Visually Evaluating Correlation



Scatter plots showing the similarity from –1 to 1.

General Approach for Combining Similarities

- Sometimes attributes are of many different types, but an overall similarity is needed.

1. For the k^{th} attribute, compute a similarity, s_k, in the range $[0, 1]$.
2. Define an indicator variable, δ_k, for the k_{th} attribute as follows:

$$\delta_k = \begin{cases} 0 & \text{if the } k^{th} \text{ attribute is a binary asymmetric attribute and both objects have} \\ & \text{a value of } 0 \text{, or if one of the objects has a missing values for the } k^{th} \text{ attribute} \\ 1 & \text{otherwise} \end{cases}$$

3. Compute the overall similarity between the two objects using the following formula:

$$similarity(p, q) = \frac{\sum_{k=1}^{n} \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.
  - Use weights w_k which are between 0 and 1 and sum to 1.

$$similarity(p, q) = \frac{\sum_{k=1}^{n} w_k \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

$$distance(p, q) = \left(\sum_{k=1}^{n} w_k |p_k - q_k|^r \right)^{1/r}.$$

Density

- Density-based clustering require a notion of density

- Examples:
    - Euclidean density
        - Euclidean density = number of points per unit volume
    - Probability density
    - Graph-based density

Euclidean Density – Cell-based

- Simplest approach is to divide region into a number of rectangular cells of equal volume and define density as # of points the cell contains

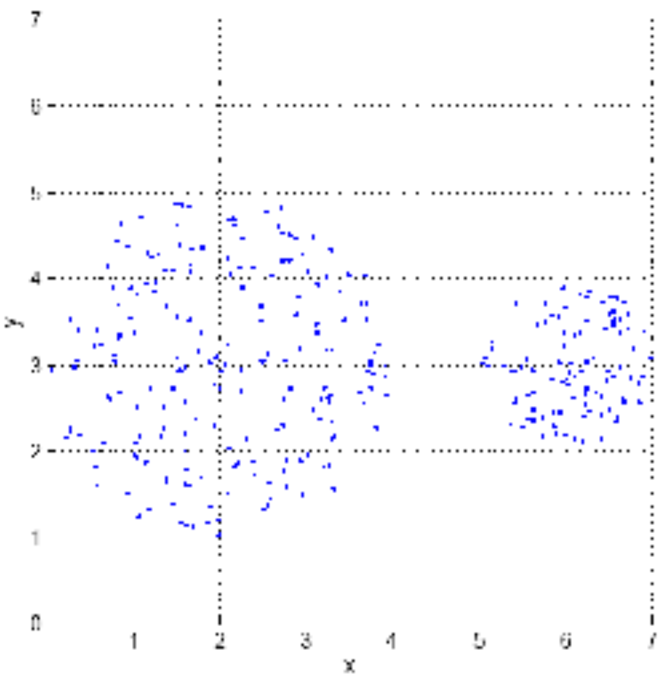


Figure 7.13. Cell-based density.

0	0	0	0	0	0	0
0	0	0	0	0	0	0
4	17	18	6	0	0	0
14	14	13	13	0	18	27
11	18	10	21	0	24	31
3	20	14	4	0	0	0
0	0	0	0	0	0	0

Table 7.6. Point counts for each grid cell.

Euclidean Density – Center-based

- Euclidean density is the number of points within a specified radius of the point

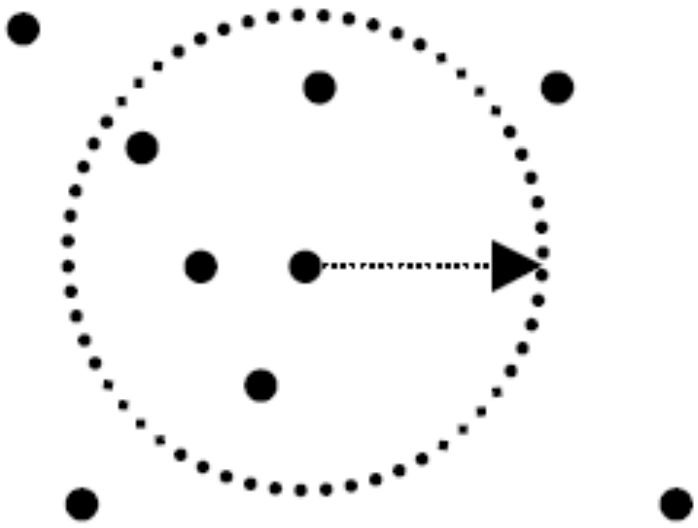


Figure 7.14. Illustration of center-based density.

Feature Subset Selection

- Another way to reduce dimensionality of data
- Redundant features
  - duplicate much or all of the information contained in one or more other attributes
  - Example: purchase price of a product and the amount of sales tax paid
- Irrelevant features
  - contain no information that is useful for the data mining task at hand
  - Example: students' ID is often irrelevant to the task of predicting students' GPA

Feature Subset Selection

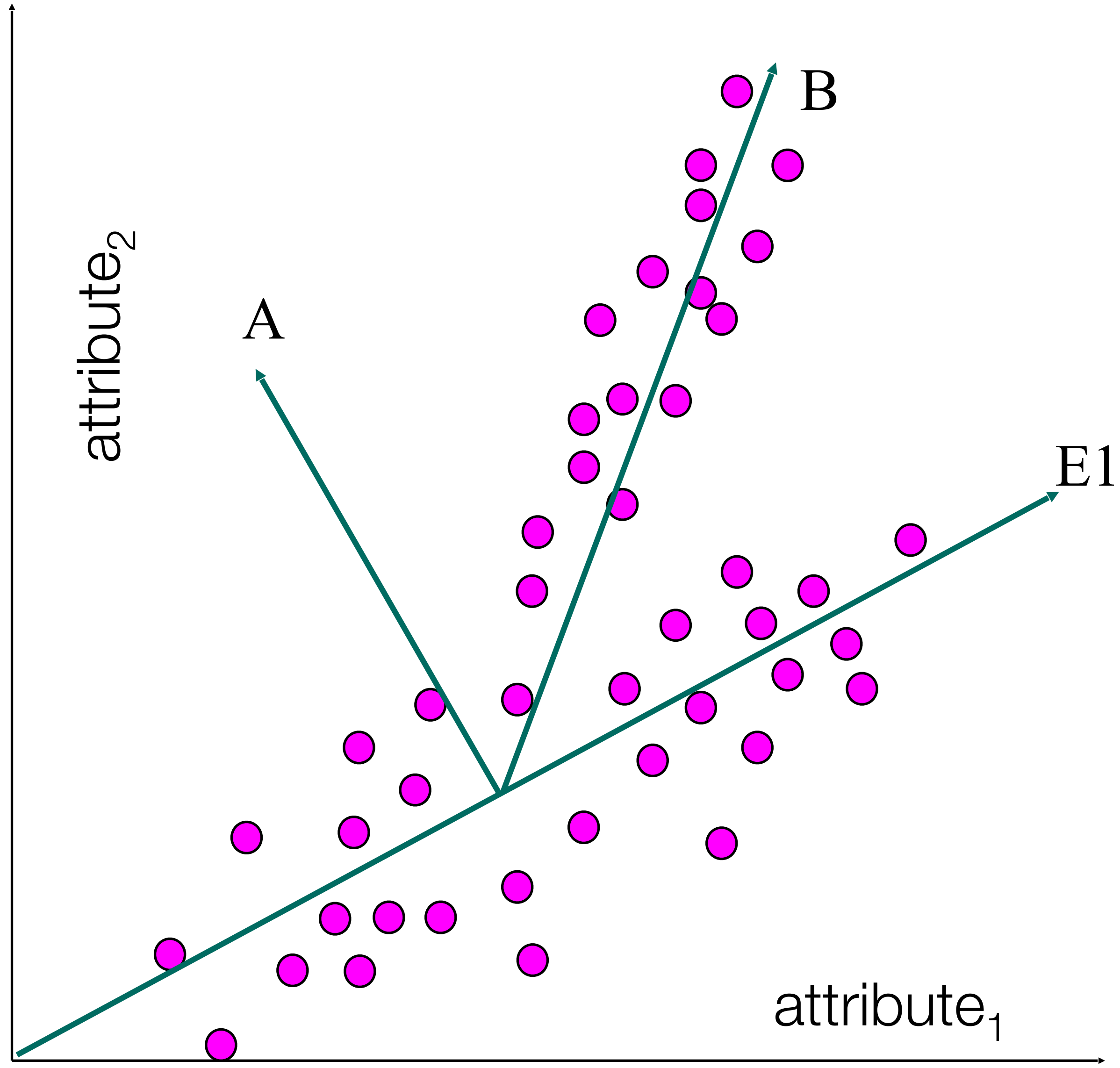
- Techniques:
  - Brute-force approch:
    - Try all possible feature subsets as input to data mining algorithm
  - Embedded approaches:
    - Feature selection occurs naturally as part of the data mining algorithm
  - Filter approaches:
    - Features are selected before data mining algorithm is run
  - Wrapper approaches:
    - Use the data mining algorithm as a black box to find best subset of attributes

Feature Creation

- Create new attributes that can capture the important information in a data set much more efficiently than the original attributes

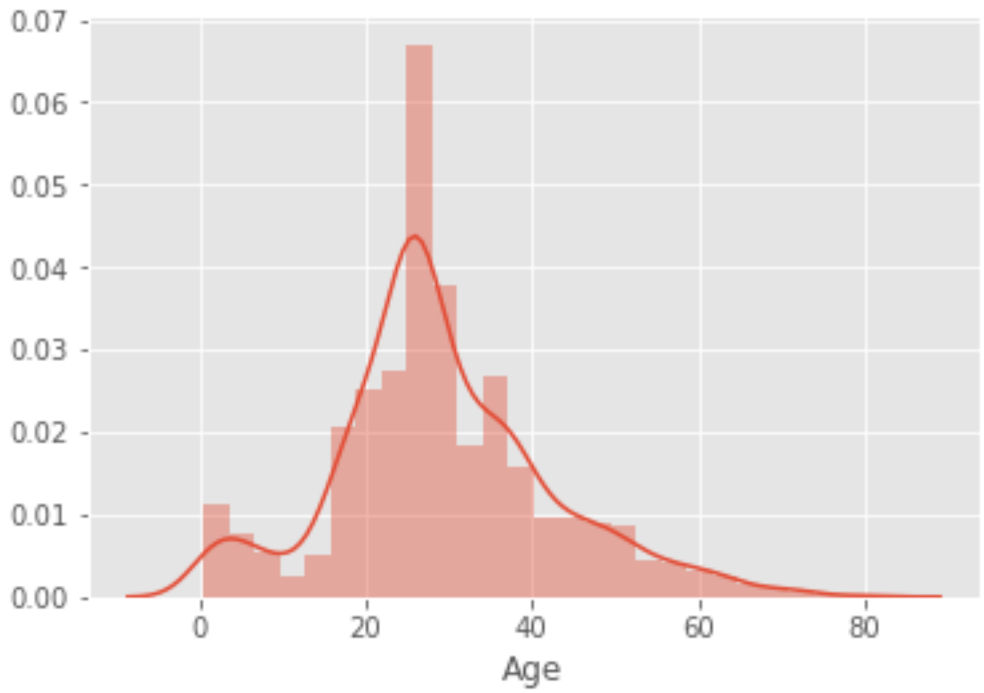
- Three general methodologies:
  - Feature Extraction
    - domain-specific
  - Mapping Data to New Space
  - Feature Construction
    - combining features

Dimensionality Reduction: PCA

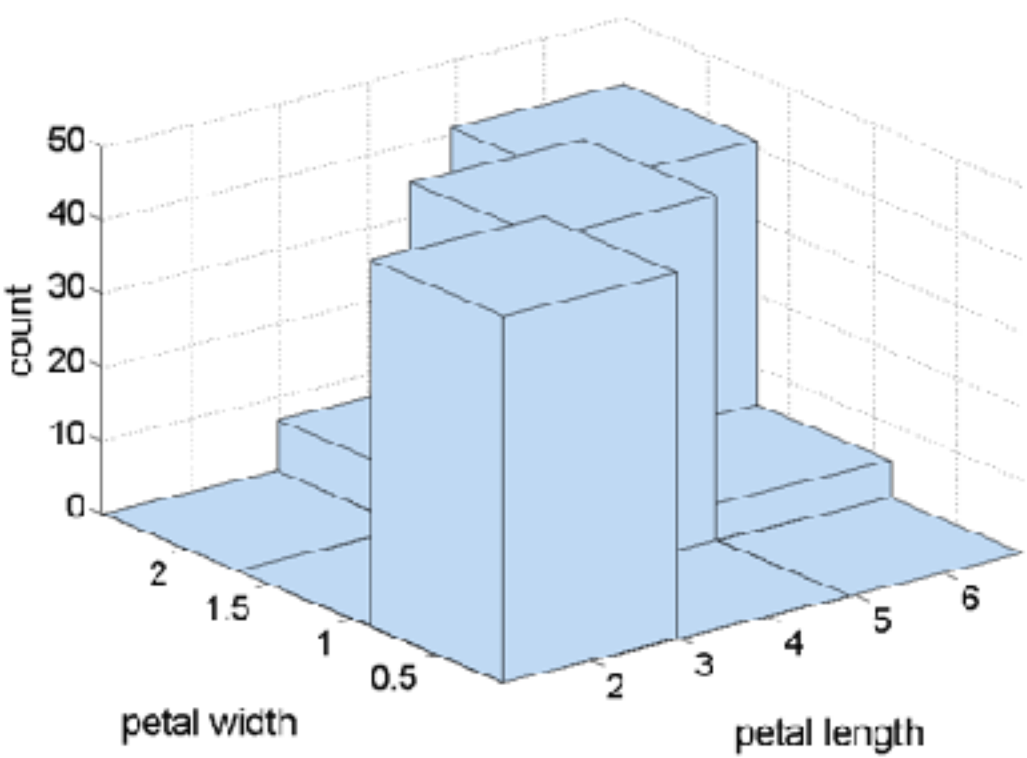


Visualization Techniques: Distributions

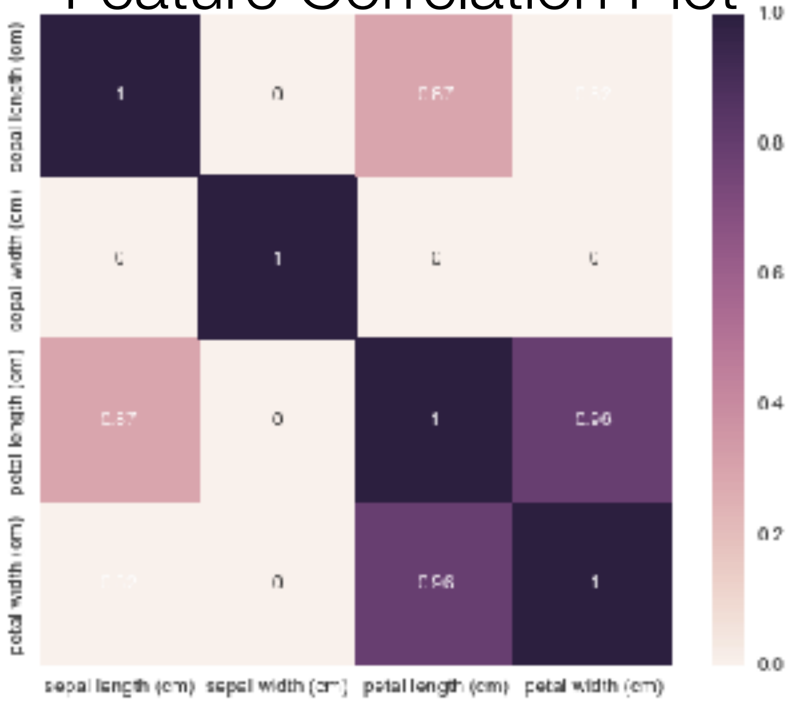
- Histogram
  - Usually shows the distribution of values of a single variable
  - Divide the values into bins and show a bar plot of the number of objects in each bin.
- KDE
  - Add up Gaussian underneath each point value
  - STD of gaussian is equivalent to number of bins in histogram



- Estimate the joint distribution of the values of two attributes
- Example: petal width and petal length
    - What does this tell us?



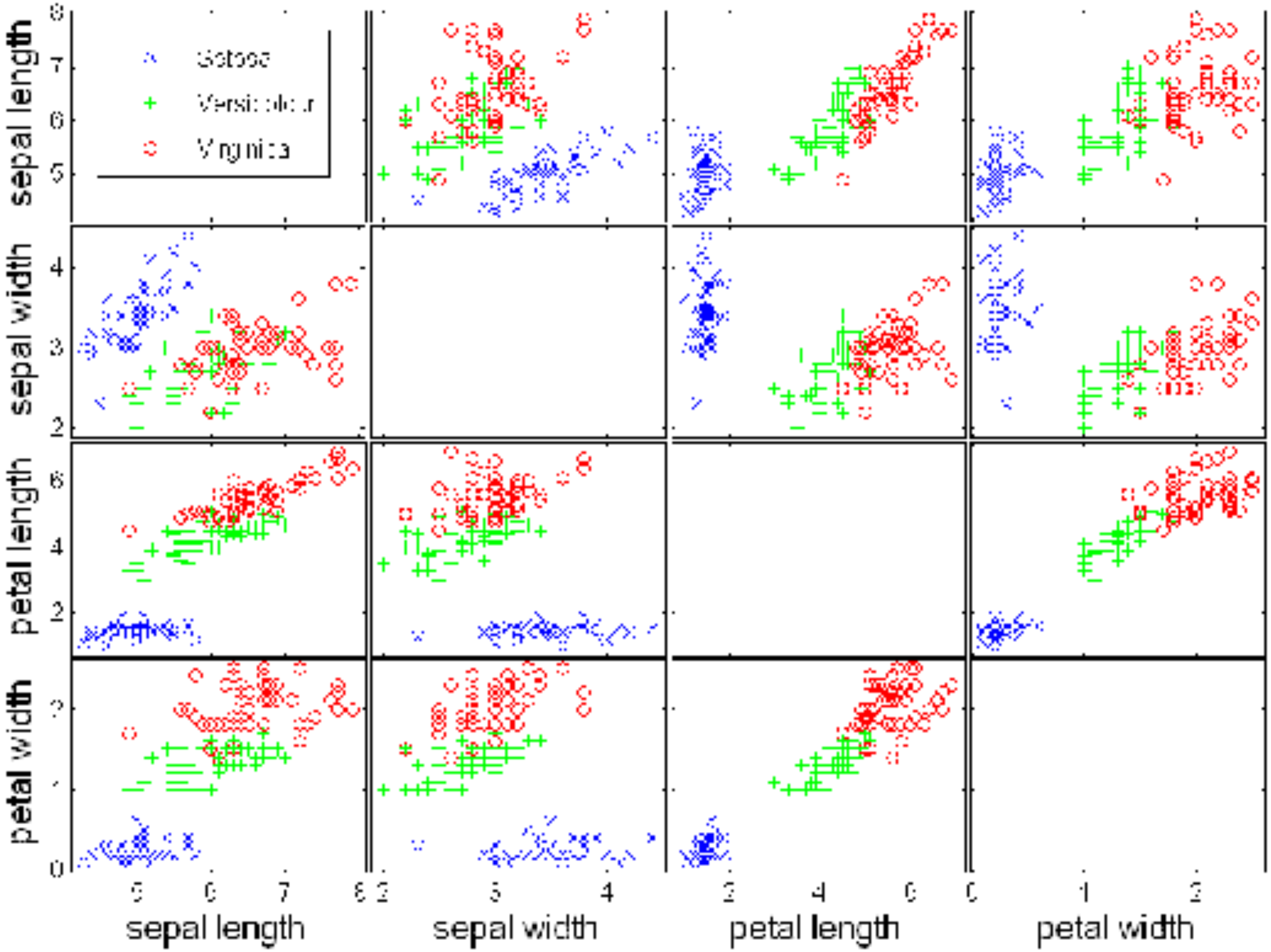
Feature Correlation Plot



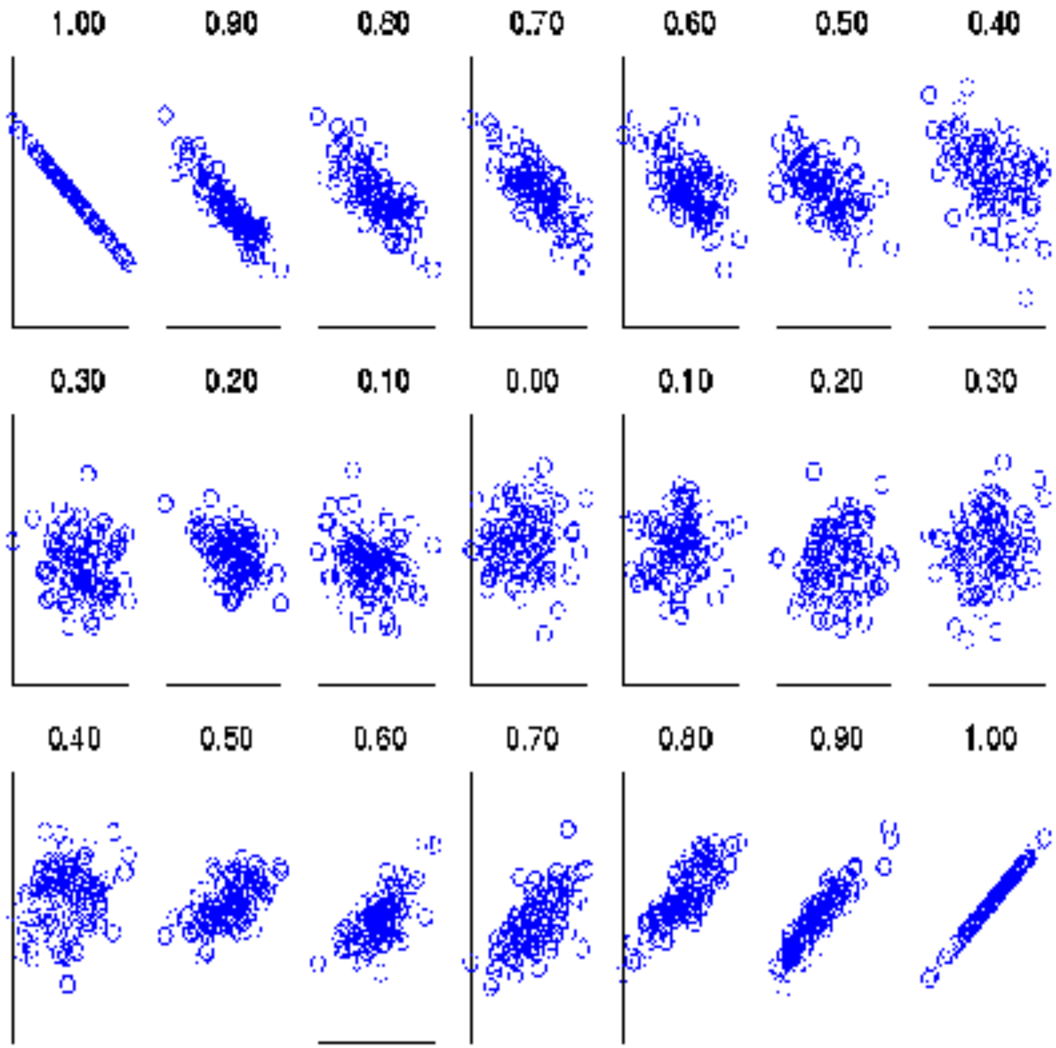
Visualization Techniques: Scatter Plots

- Scatter plots
  - Two-dimensional scatter plots most common
  - **Additional attributes** can be displayed by using the **size, shape, and color** of the markers that represent the objects
  - **Interactivity** can add **insight**
  - It is useful to have **matrices of scatter plots** to compactly summarize the relationships of several pairs of attributes
  - Good for numeric data, but needs **jitter** for categorical data

Scatter Plot Matrix Colored by Class



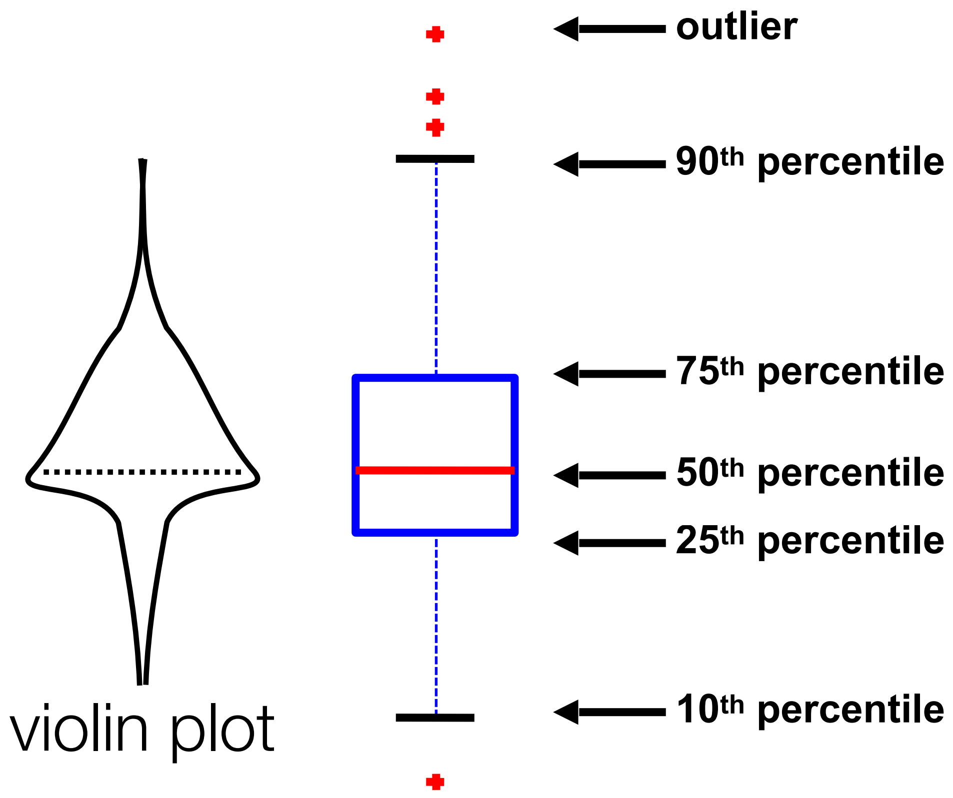
Visually Evaluating Correlation



Scatter plots showing the similarity from –1 to 1.

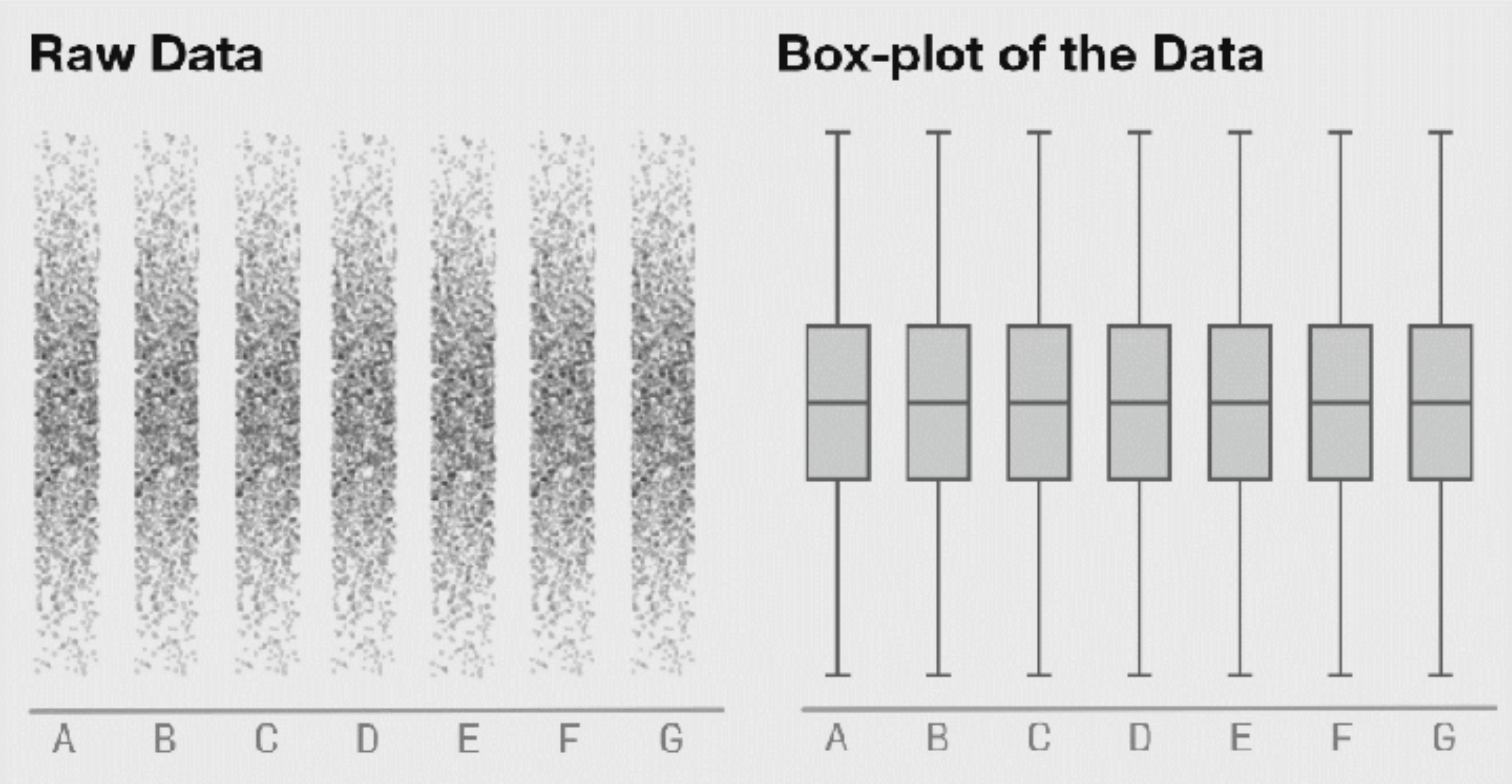
Visualization Techniques: Box Plots

- Box Plots
  - Invented by J. Tukey
  - Another way of displaying the distribution of data
  - Following figure shows the basic part of a box plot



Visualization Techniques: Box Plots

- Box Plots

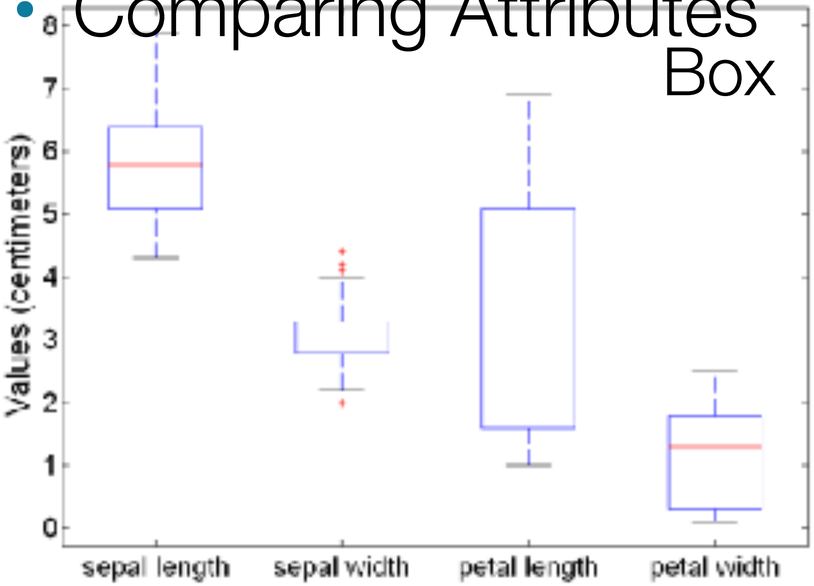


https://www.reddit.com/r/dataisbeautiful/comments/6ssmzc/be_wary_of_boxplots_they_could_be_hiding/

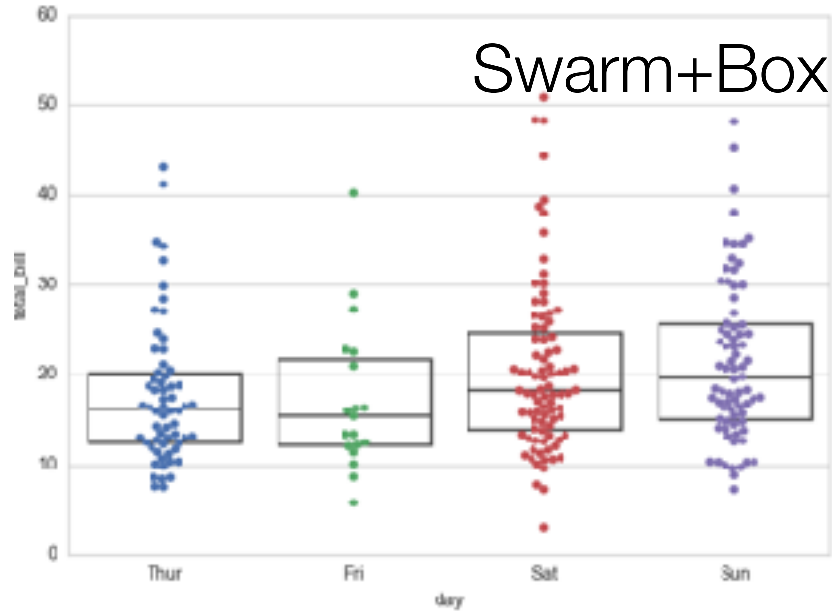
Example: Comparing Attributes

- Comparing Attributes

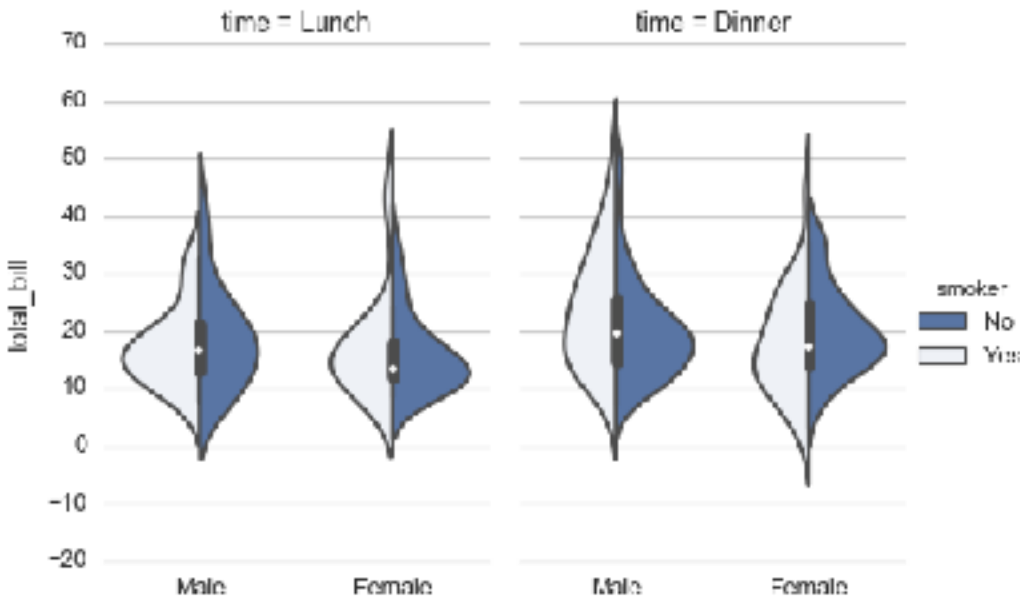
Box



Swarm+Box



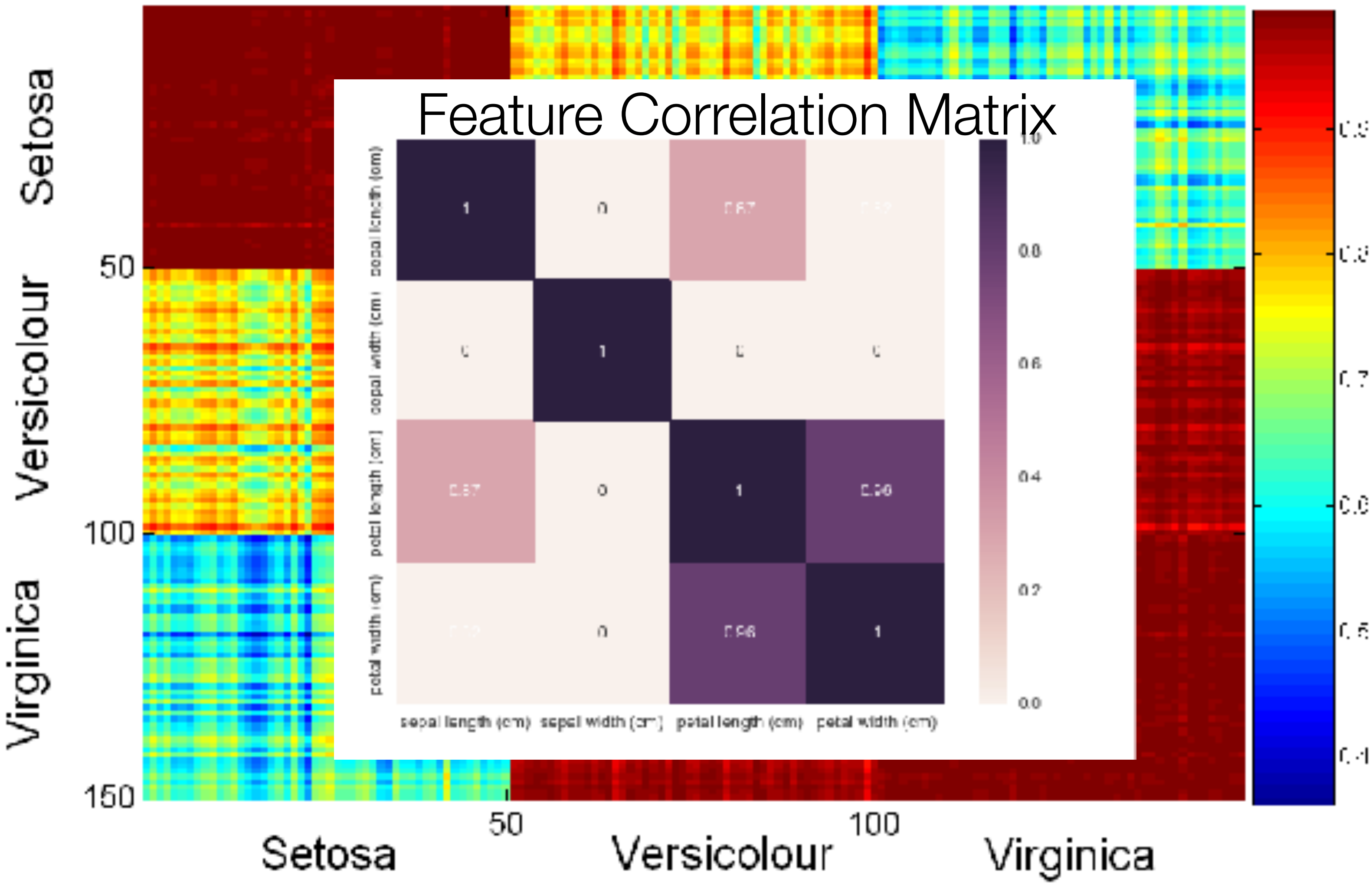
Mixed Violin + Box



Visualization Techniques: Matrix Plots

- Matrix plots (typically heatmaps)
  - Plot some data matrix
  - This can be useful when objects are sorted well
  - Typically, the attributes are normalized to prevent one attribute from dominating the plot
  - Plots of similarity or distance matrices can also be useful for visualizing the relationships between objects

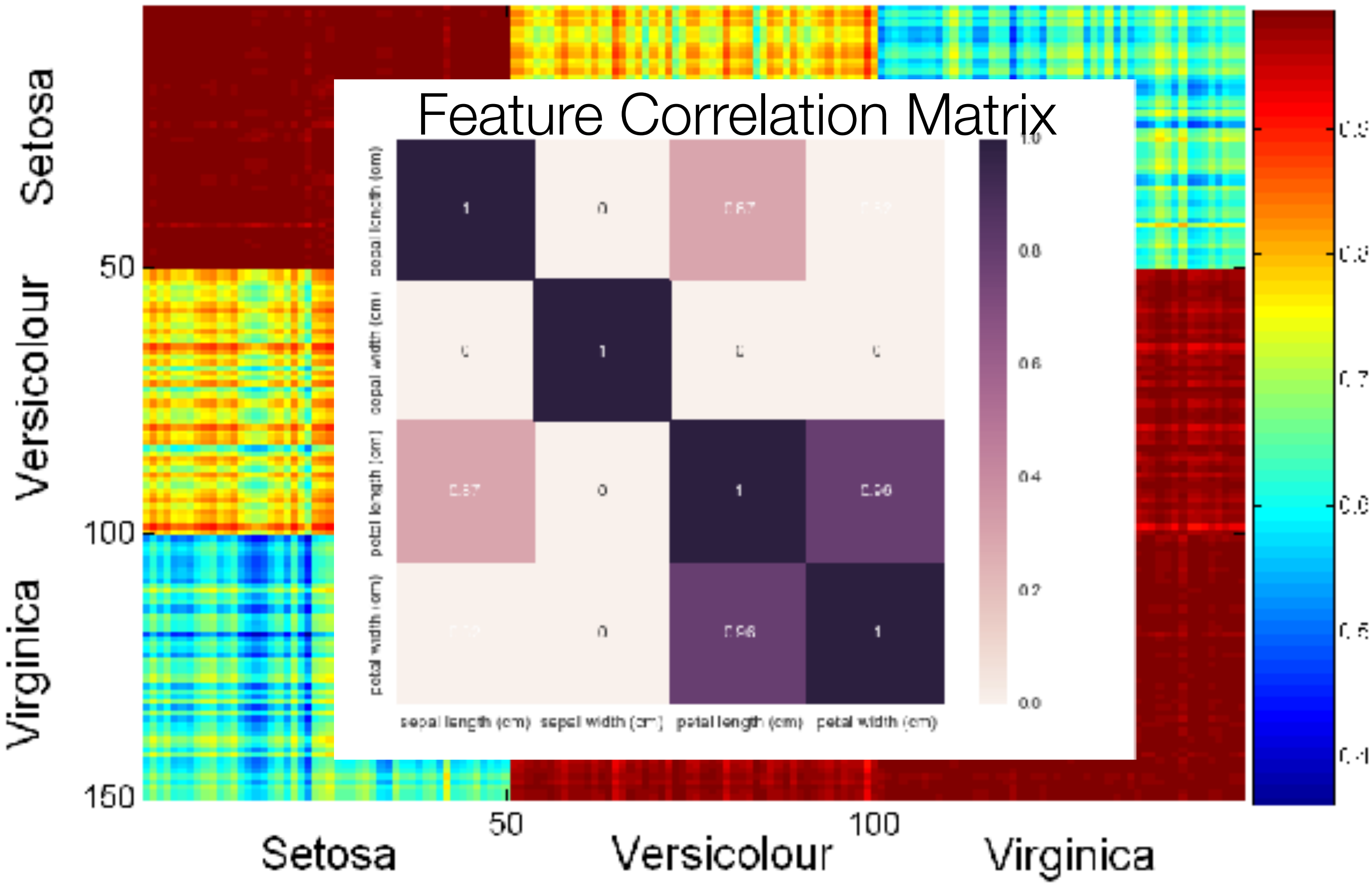
Instance Correlation Matrix



Visualization Techniques: Matrix Plots

- Matrix plots (typically heatmaps)
  - Plot some data matrix
  - This can be useful when objects are sorted well
  - Typically, the attributes are normalized to prevent one attribute from dominating the plot
  - Plots of similarity or distance matrices can also be useful for visualizing the relationships between objects

Instance Correlation Matrix



Visualization Techniques: Parallel Coordinates

- Parallel Coordinates
  - Used to plot the attribute values of multi-dimensional data
  - Instead of using perpendicular axes, use a set of parallel axes
  - The attribute values of each object are plotted as a point on each corresponding coordinate axis and the points are connected by a line
  - Thus, each object is represented as a line
  - Often, the lines representing a distinct class of objects group together, at least for some attributes
  - Ordering of attributes is important in seeing such groupings

Parallel Coordinates Plots for Iris Data