FDSA

About Data

Material Adaptation from Introduction to Data Mining : Tan, Steinbach, Karpatne, Kumar

Outline

- Attributes and Objects
- Types of Data
- Data Quality
- Similarity and Distance
- Data Preprocessing

Data : Distinction

- Data
- Information
- Knowledge

Data : Distinction

- Data
- Information
- Knowledge

12 , 34 , 16 , 32, 18, 35

What are these ?

Data ? Information ?

Data : Distinction

- Data
- Information
- Knowledge

Last Three days
(June 3,4,5)
Min – Max Temp of
Kathmandu

12 , 34 , 16 , 32, 18, 35

What are these ?

Data ? Information ?
Knowledge ?

Data : Distinction

- Data
- Information
- Knowledge

Last Three days
Min – Max Temp of
Kathmandu

12 , 34 , 16 , 32, 18, 35

Average Temp ?
23, 24, 26.5

Data : Distinction

- Data
- Information
- Knowledge

Last Three days (June 3,4,5)
Min – Max Temp of Kathmandu

12 , 34 , 16 , 32, 18, 35

A traveler seeks Knowledge regarding traveling to KTM in the month of June!

Whether Jacket is needed or not if the travel is during the month of June ?

What is Data?

- Collection of ***data objects*** and their ***attributes***
- An ***attribute*** is a property or characteristic of an object
  - Examples: eye color of a person, temperature, etc.
  - Attribute is also known as variable, field, characteristic, dimension, or feature
- A collection of attributes describe an ***object***
  - Object is also known as record, point, case, sample, entity, or instance

Attributes

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Objects

Attribute Values

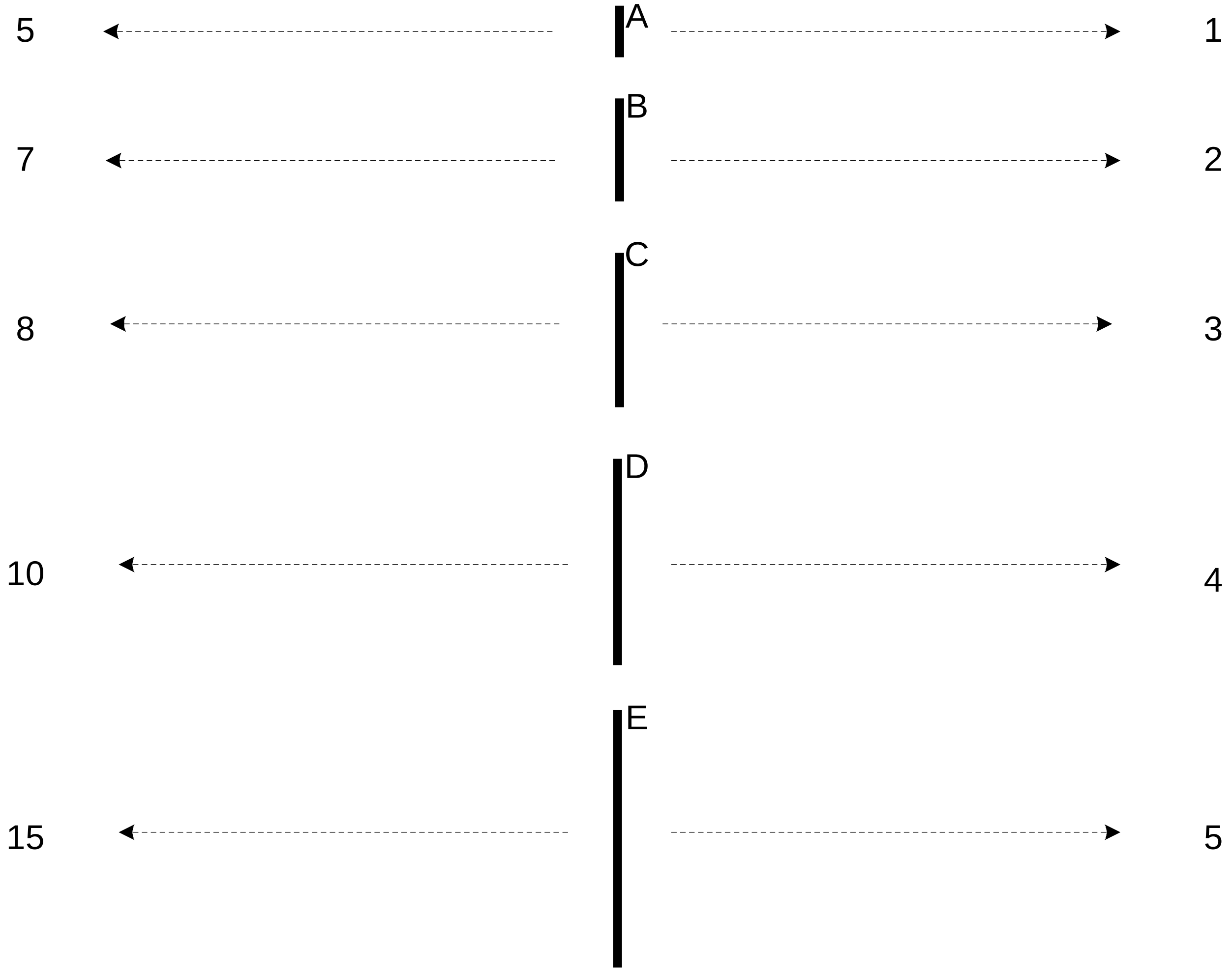
- ***Attribute values*** are numbers or symbols assigned to an attribute for a particular object

- Distinction between attributes and attribute values
  - Same attribute can be mapped to different attribute values
    - Example: height can be measured in feet or meters
  - Different attributes can be mapped to the same set of values
    - Example: Attribute values for ID and age are integers
    - But properties of attribute values can be different

Measurement of Length

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

This scale preserves only the ordering property of length.



This scale preserves the ordering and additivity properties of length.

Types of Attributes

- There are different types of attributes
  - Nominal
    - Examples: ID numbers, eye color, zip codes
  - Ordinal
    - Examples: rankings (e.g., taste of potato chips on a scale from 1-10), grades, height {tall, medium, short}
  - Interval
    - Examples: calendar dates, temperatures in Celsius or Fahrenheit.
  - Ratio
    - Examples: temperature in Kelvin, length, time, counts

Properties of Attribute Values

- The type of an attribute depends on which of the following properties/operations it possesses:

– Distinctness:	= ≠
– Order:	< >
– Differences are meaningful :	+ -
– Ratios are meaningful	* /

  - Nominal attribute: distinctness
  - Ordinal attribute: distinctness & order
  - Interval attribute: distinctness, order & meaningful differences
  - Ratio attribute: all 4 properties/operations

Difference Between Ratio and Interval

- Is it physically meaningful to say that a temperature of 10 ° is twice that of 5° on
  - the Celsius scale?
  - the Fahrenheit scale?
  - the Kelvin scale?

- The meaning of 0 (Zero) difference
  - Last night temp reached up to 0 ° C
  - As a full-time student, he is earning 0 Rs per month!

	Attribute Type	Description	Examples	Operations
Categorical Qualitative	Nominal	Nominal attribute values only distinguish. (=, ≠)	zip codes, employee ID numbers, eye color, sex: {*male, female*}	mode, entropy, contingency correlation, χ2 test
	Ordinal	Ordinal attribute values also order objects. (<, >)	hardness of minerals, {*good, better, best*}, grades, street numbers	median, percentiles, rank correlation, run tests, sign tests
Numeric Quantitative	Interval	For interval attributes, differences between values are meaningful. (+, -)	calendar dates, temperature in Celsius or Fahrenheit	mean, standard deviation, Pearson's correlation, *t* and *F* tests
	Ratio	For ratio variables, both differences and ratios are meaningful. (*, /)	temperature in Kelvin, monetary quantities, counts, age, mass, length, current	geometric mean, harmonic mean, percent variation

This categorization of attributes is due to S. S. Stevens

	Attribute Type	**Transformation**	**Comments**
Categorical Qualitative	Nominal	Any permutation of values	If all employee ID numbers were reassigned, would it make any difference?
	Ordinal	An order preserving change of values, i.e., *new_value = f(old_value)* where *f* is a monotonic function	An attribute encompassing the notion of good, better best can be represented equally well by the values {1, 2, 3} or by { 0.5, 1, 10}.
Numeric Quantitative	Interval	*new_value = a * old_value + b* where a and b are constants	Thus, the Fahrenheit and Celsius temperature scales differ in terms of where their zero value is and the size of a unit (degree).
	Ratio	*new_value = a * old_value*	Length can be measured in meters or feet.

This categorization of attributes is due to S. S. Stevens

Discrete and Continuous Attributes

- Discrete Attribute
  - Has only a finite or countably infinite set of values
  - Examples: zip codes, counts, or the set of words in a collection of documents
  - Often represented as integer variables.
  - Note: binary attributes are a special case of discrete attributes
- Continuous Attribute
  - Has real numbers as attribute values
  - Examples: temperature, height, or weight.
  - Practically, real values can only be measured and represented using a finite number of digits.
  - Continuous attributes are typically represented as floating-point variables.

Asymmetric Attributes

- Only presence (a non-zero attribute value) is regarded as important
  - Words present in documents
  - Items present in customer transactions

- If we met a friend in the grocery store would we ever say the following?

  "I see our purchases are very similar since we didn't buy most of the same things."

- Asymmetric attributes typically arise from objects that are sets

- We need two asymmetric binary attributes to represent one ordinary binary attribute
  - Association analysis uses asymmetric attributes

Types of data sets (Organization Aspect)

- Record
  - Data Matrix
  - Document Data
  - Transaction Data
- Graph
  - World Wide Web
  - Molecular Structures
- Ordered
  - Spatial Data
  - Temporal Data
  - Sequential Data
  - Genetic Sequence Data

Record Data

- Data that consists of a collection of records, each of which consists of a fixed set of attributes

Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	**No**
2	No	Married	100K	**No**
3	No	Single	70K	**No**
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5	No	Divorced	95K	**Yes**
6	No	Married	60K	**No**
7	Yes	Divorced	220K	**No**
8	No	Single	85K	**Yes**
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10	No	Single	90K	**Yes**

Data Matrix

- If data objects have the same fixed set of numeric attributes, then the data objects can be thought of as points in a multi-dimensional space, where each dimension represents a distinct attribute

- Such data set can be represented by an *m* by *n* matrix, where there are *m* rows, one for each object, and *n* columns, one for each attribute

Projection of x Load	**Projection of y load**	**Distance**	**Load**	**Thickness**
10.23	5.27	15.22	2.7	1.2
12.65	6.25	16.22	2.2	1.1

Document Data

- Each document becomes a ‘term’ vector
  - Each term is a component (attribute) of the vector
  - The value of each component is the number of times the corresponding term occurs in the document.

	team	coach	play	ball	score	game	win	lost	timeout	season
Document 1	3	0	5	0	2	6	0	2	0	2
Document 2	0	7	0	2	1	0	0	3	0	0
Document 3	0	1	0	0	1	2	2	0	3	0

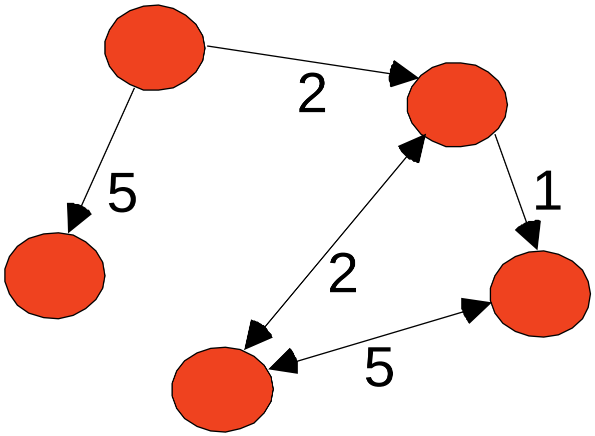
Transaction Data

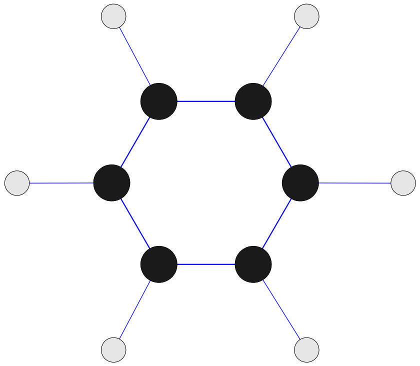
- A special type of record data, where
  - Each record (transaction) involves a set of items.
  - For example, consider a grocery store. The set of products purchased by a customer during one shopping trip constitute a transaction, while the individual products that were purchased are the items.

TID	*Items*
1	**Bread, Coke, Milk**
2	**Beer, Bread**
3	**Beer, Coke, Diaper, Milk**
4	**Beer, Bread, Diaper, Milk**
5	**Coke, Diaper, Milk**

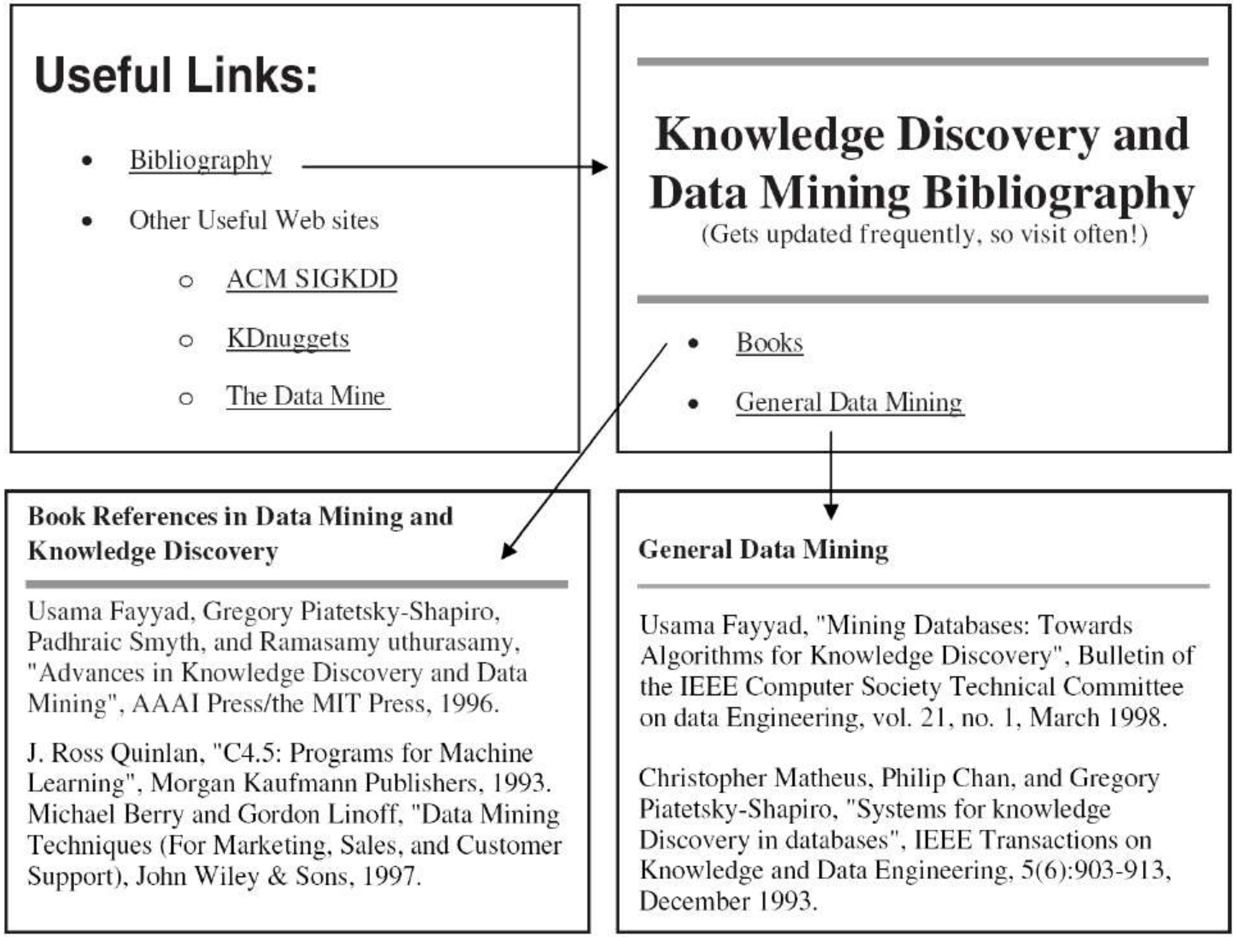
Graph Data

- Examples: Generic graph, a molecule, and webpages





Benzene Molecule: C6H6



Useful Links:

- Bibliography
- Other Useful Web sites
  - ACM SIGKDD
  - KDnuggets
  - The Data Mine

Knowledge Discovery and Data Mining Bibliography

(Gets updated frequently, so visit often!)

- Books
- General Data Mining

Book References in Data Mining and Knowledge Discovery

Usama Fayyad, Gregory Piatetsky-Shapiro, Padhraic Smyth, and Ramasamy uthurasamy, "Advances in Knowledge Discovery and Data Mining", AAAI Press/the MIT Press, 1996.

J. Ross Quinlan, "C4.5: Programs for Machine Learning", Morgan Kaufmann Publishers, 1993. Michael Berry and Gordon Linoff, "Data Mining Techniques (For Marketing, Sales, and Customer Support), John Wiley & Sons, 1997.

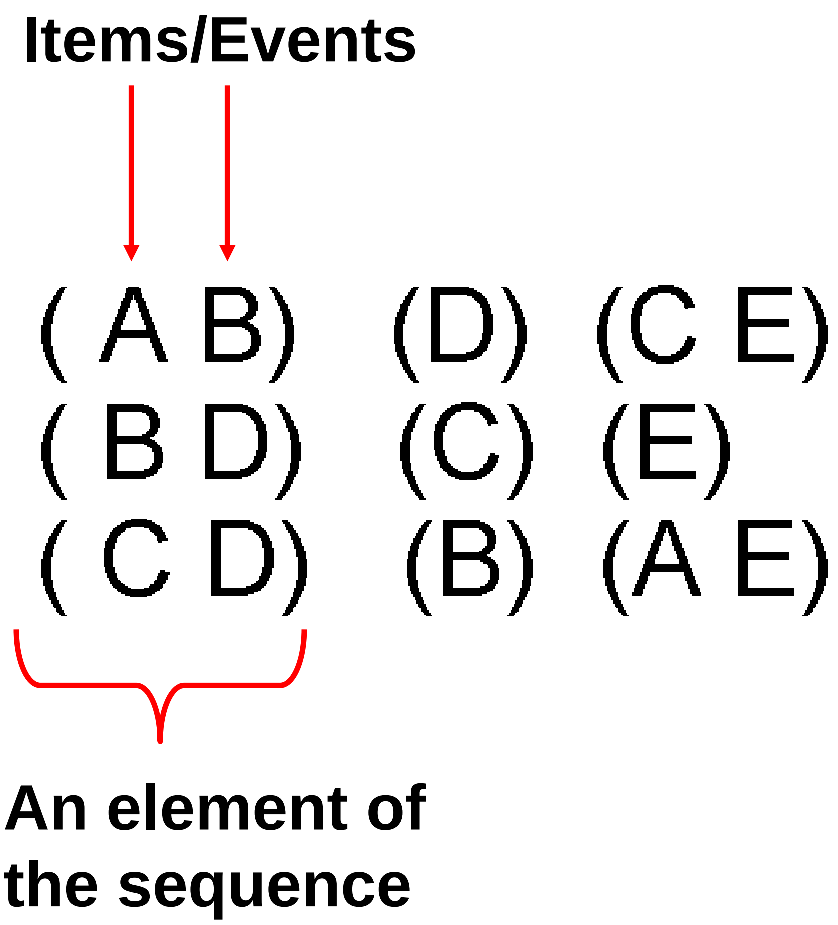
General Data Mining

Usama Fayyad, "Mining Databases: Towards Algorithms for Knowledge Discovery", Bulletin of the IEEE Computer Society Technical Committee on data Engineering, vol. 21, no. 1, March 1998.

Christopher Matheus, Philip Chan, and Gregory Piatetsky-Shapiro, "Systems for knowledge Discovery in databases", IEEE Transactions on Knowledge and Data Engineering, 5(6):903-913, December 1993.

Ordered Data

- Sequences of transactions



Items/Events

(A B) (D) (C E)

(B D) (C) (E)

(C D) (B) (A E)

An element of the sequence

Ordered Data

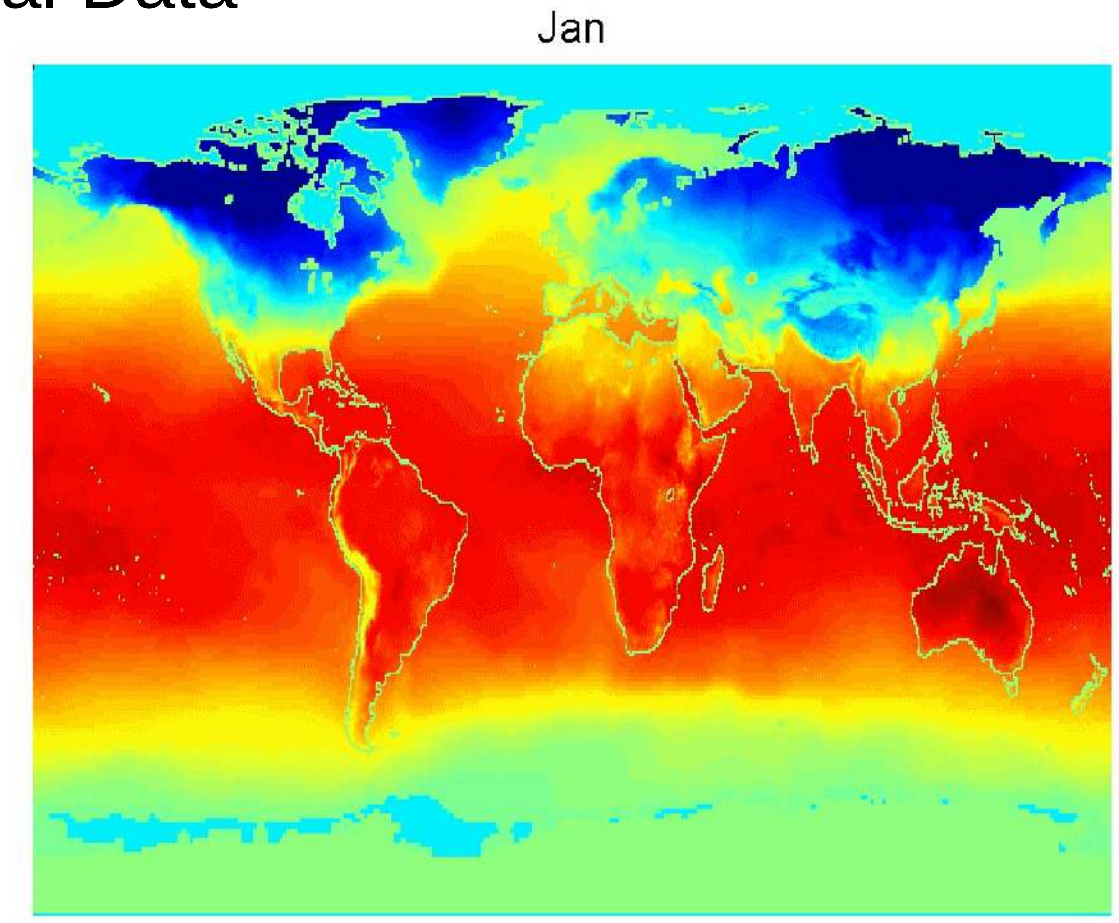
- Genomic sequence data

```
GGTTCCGCCTTCAGCCCCGCGCC
CGCAGGGCCCGCCCCGCGCCGTC
GAGAAGGGCCCGCCTGGCGGGCG
GGGGGAGGCGGGGCCGCCCGAGC
CCAACCGAGTCCGACCAGGTGCC
CCCTCTGCTCGGCCTAGACCTGA
GCTCATTAGGCGGCAGCGGACAG
GCCAAGTAGAACACGCGAAGCGC
TGGGCTGCCTGCTGCGACCAGGG
```

Ordered Data

- Spatio-Temporal Data

Average Monthly Temperature of land and ocean



Important Characteristics of Data

- Dimensionality (number of attributes)
  - High dimensional data brings a number of challenges

- Sparsity
  - Only presence counts

- Resolution
  - Patterns depend on the scale

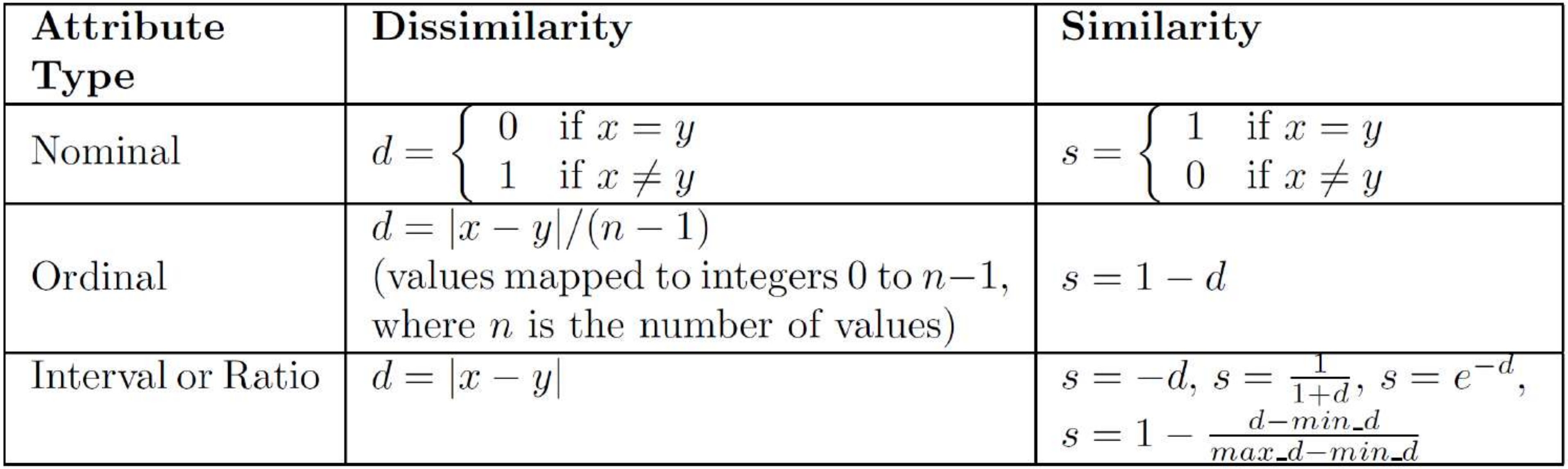
- Size
  - Type of analysis may depend on size of data

Similarity and Dissimilarity Measures

- Similarity measure
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- Dissimilarity measure
  - Numerical measure of how different two data objects are
  - 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

The following table shows the similarity and dissimilarity between two objects, *x* and *y*, with respect to a single, simple attribute.



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

Euclidean Distance

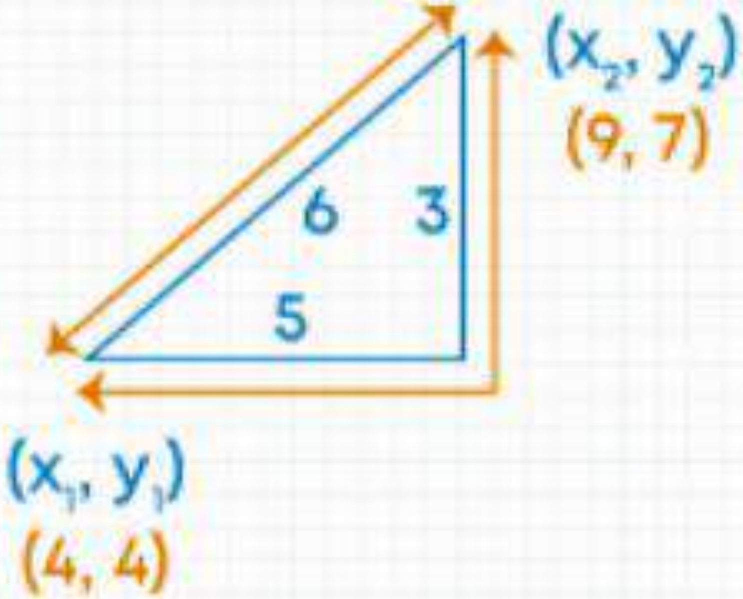
- Euclidean Distance

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{k=1}^{n} (x_k - y_k)^2}$$

where *n* is the number of dimensions (attributes) and x_k and y_k are, respectively, the k^{th} attributes (components) or data objects $\mathbf{x}$ and $\mathbf{y}$.

- Standardization is necessary, if scales differ.

Example:



Euclidean distance

$$= \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

$$= \sqrt{(9 - 4)^2 + (7 - 4)^2}$$

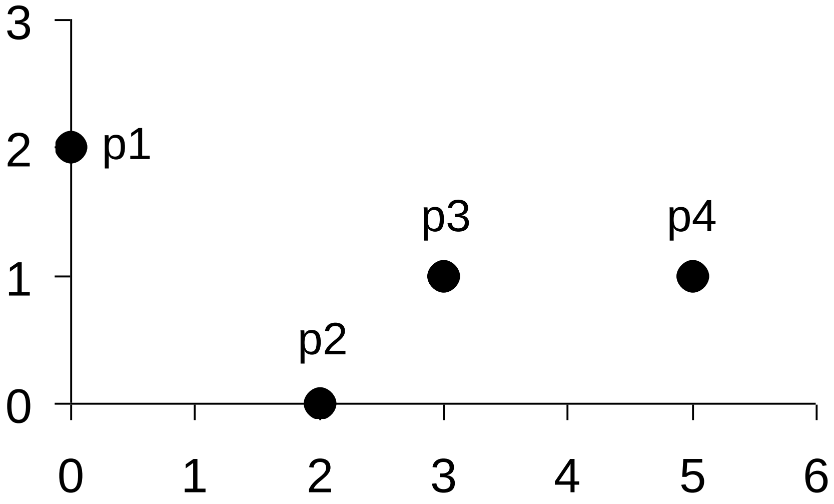
$$= \sqrt{5^2 + 3^2}$$

$$= \sqrt{25 + 9}$$

$$= \sqrt{34}$$

$$= 5.83$$

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

$$d(\mathbf{x}, \mathbf{y}) = \left(\sum_{k=1}^{n} |x_k - y_k|^r \right)^{1/r}$$

Where r is a parameter, n is the number of dimensions (attributes) and x_k and y_k are, respectively, the k^{th} attributes (components) or data objects $\boldsymbol{x}$ and $\boldsymbol{y}$.

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

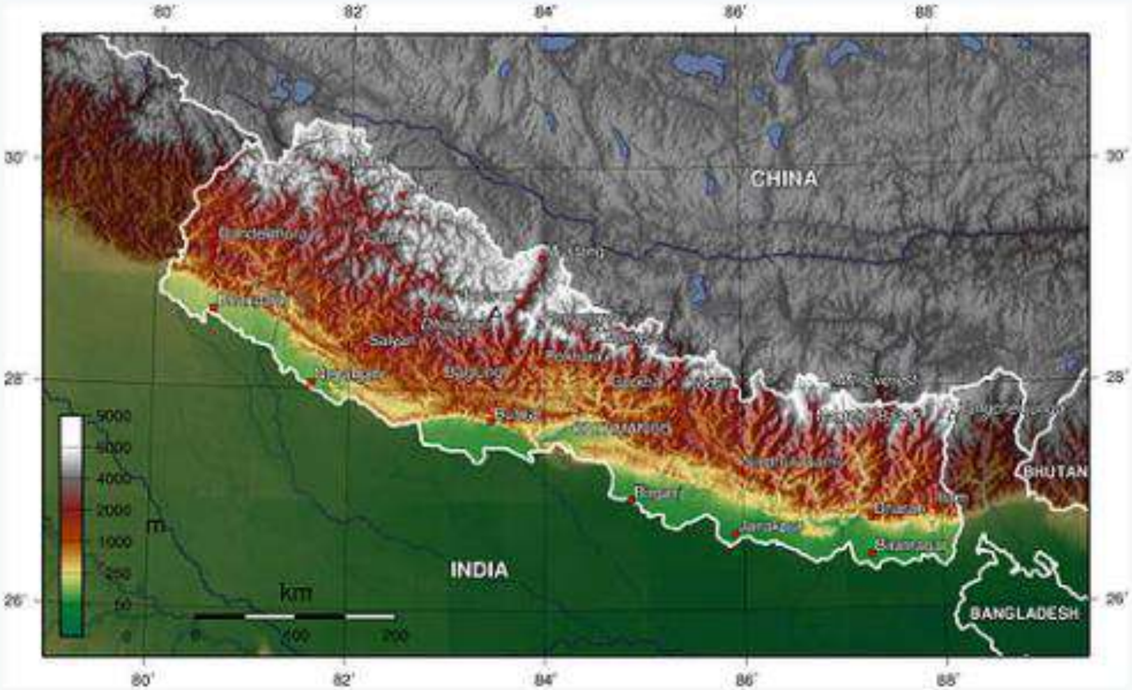
- *r* = 2. Euclidean distance

- $r \rightarrow \infty$. "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.

Nepal measures about 880 kilometers (547 mi) along its Himalayan axis by 150 to 250 kilometers (93 to 155 mi) across. It has an area of 147,516 km^2 (56,956 sq mi).[1]

Geography of Nepal (नेपाल)



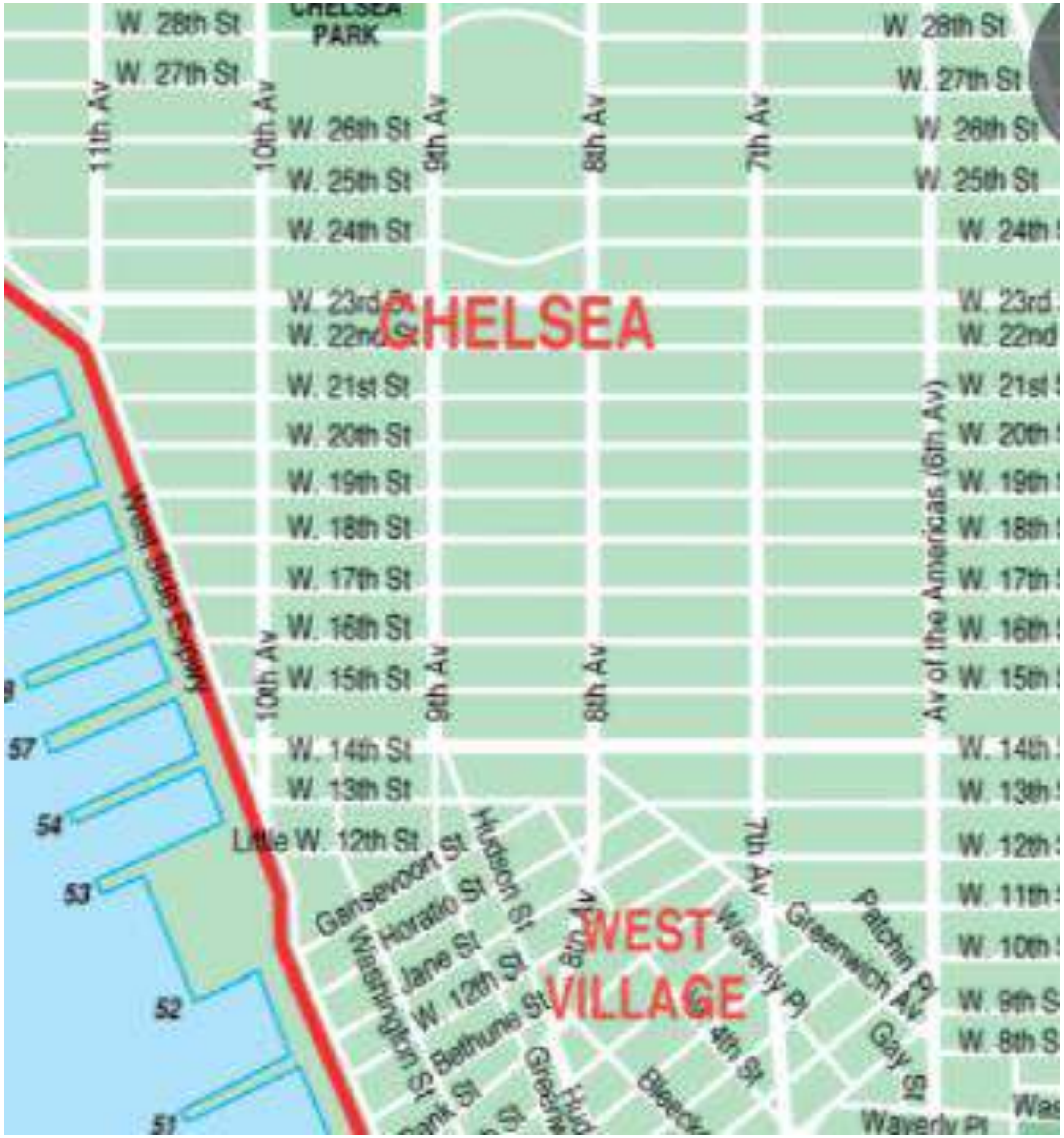
Continent	Asia

1027.67 km

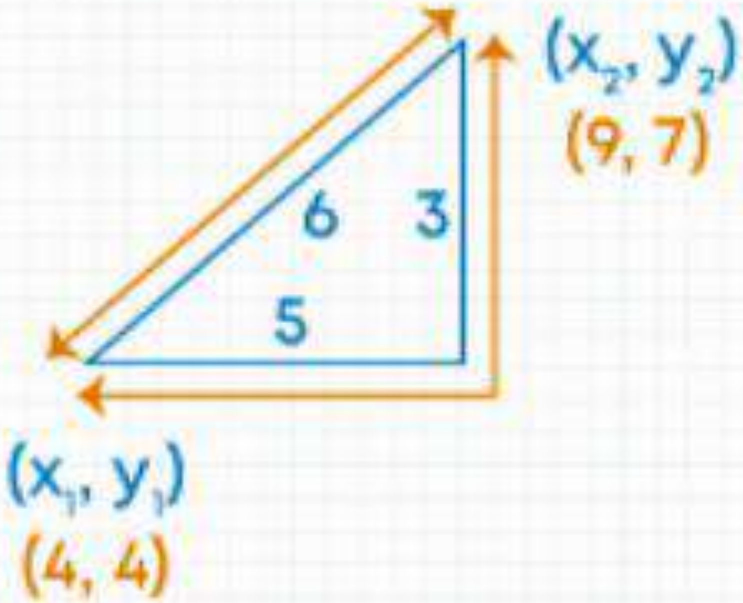
East west Highway of **Nepal** is also known as the Mahendra **highway** is the longest roadway

Length of **east-west highway** is 1027.67 km. Feb 23, 2016

Manhattan Street Map



Example:



Euclidean distance

$$= \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

$$= \sqrt{(9 - 4)^2 + (7 - 4)^2}$$

$$= \sqrt{5^2 + 3^2}$$

$$= \sqrt{25 + 9}$$

$$= \sqrt{34}$$

$$= 5.83$$

Manhattan distance

$$= |x_2 - x_1| + |y_2 - y_1|$$

$$= |9 - 4| + |7 - 4|$$

$$= 5 + 3$$

$$= 8$$

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

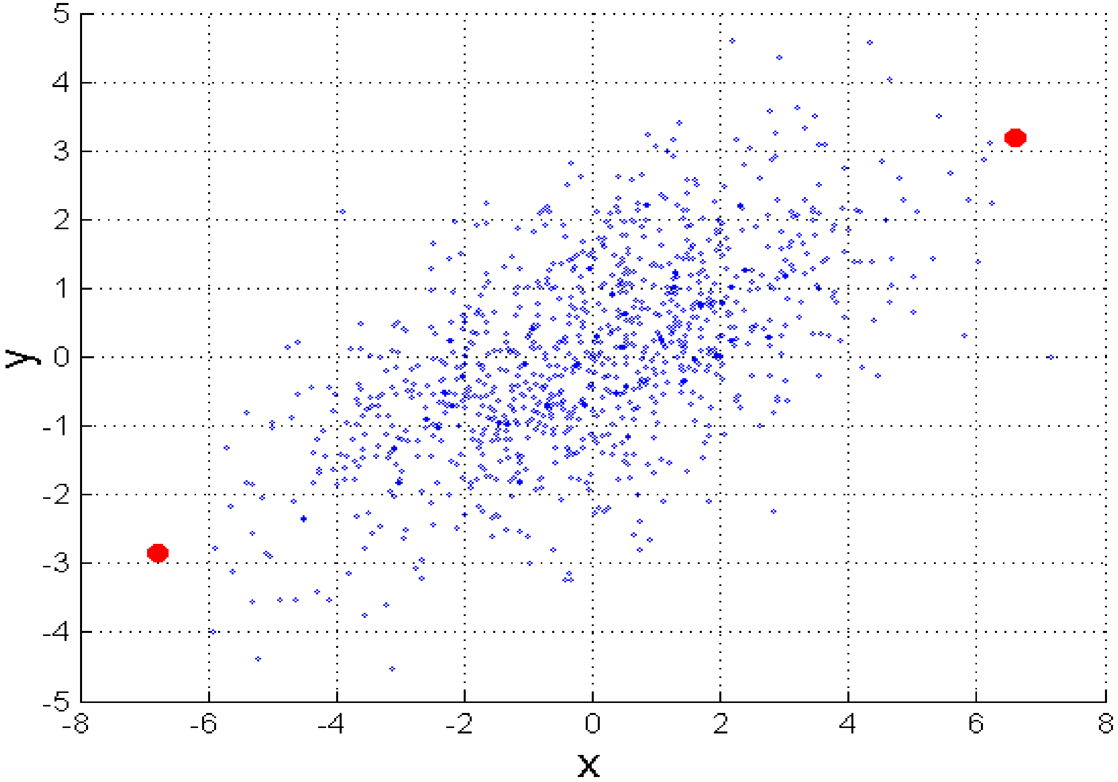
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

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

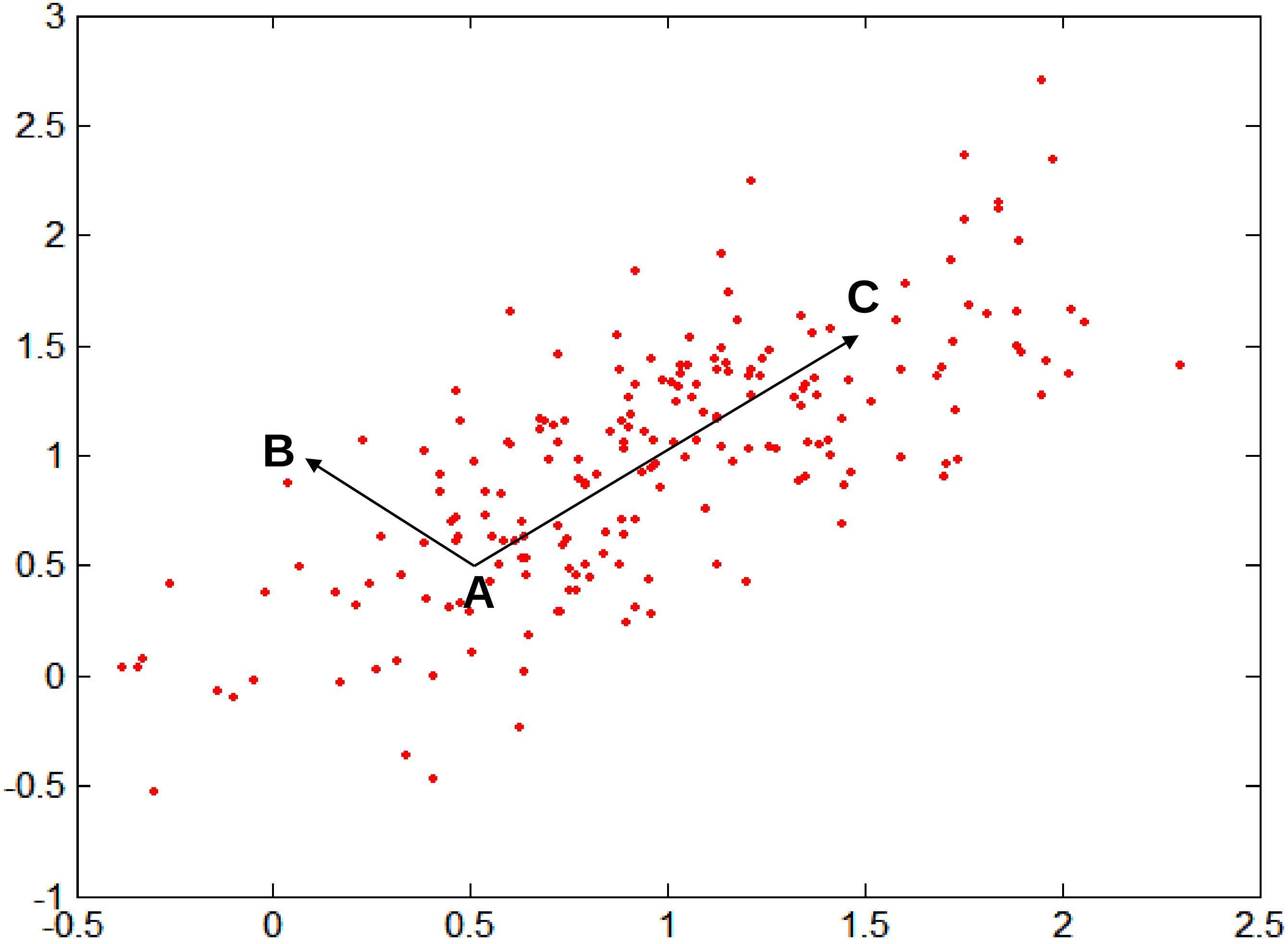
$$\mathbf{mahalanobis}(\mathbf{x}, \mathbf{y}) = (\mathbf{x} - \mathbf{y})^T\, \Sigma^{-1}(\mathbf{x} - \mathbf{y})$$



Σ is the covariance matrix

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

Similarity Between Binary Vectors

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

- Compute similarities using the following quantities

  f_{01} = the number of attributes where *p* was 0 and *q* was 1

  f_{10} = the number of attributes where *p* was 1 and *q* was 0

  f_{00} = the number of attributes where *p* was 0 and *q* was 0

  f_{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

  $= (f_{11} + f_{00}) / (f_{01} + f_{10} + f_{11} + f_{00})$

  J = number of 11 matches / number of non-zero attributes

  $= (f_{11}) / (f_{01} + f_{10} + f_{11})$

SMC versus Jaccard: Example

$\mathbf{x} =$ 1 0 0 0 0 0 0 0 0 0

$\mathbf{y} =$ 0 0 0 0 0 0 1 0 0 1

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

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

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

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

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

$$\text{J} = (f_{11}) / (f_{01} + f_{10} + f_{11}) = 0 / (2 + 1 + 0) = 0$$

Cosine Similarity

- If $\mathbf{d}_1$ and $\mathbf{d}_2$ are two document vectors, then

$$\cos(\mathbf{d}_1, \mathbf{d}_2) = \langle \mathbf{d}_1,\mathbf{d}_2 \rangle / \|\mathbf{d}_1\| \, \|\mathbf{d}_2\| ,$$

where $\langle \mathbf{d}_1,\mathbf{d}_2 \rangle$ indicates inner product or vector dot product of vectors, $\mathbf{d}_1$ and $\mathbf{d}_2$, and $\| \mathbf{d} \|$ is the length of vector $\mathbf{d}$.

- Example:

$$\mathbf{d}_1 = \mathbf{3\ 2\ 0\ 5\ 0\ 0\ 0\ 2\ 0\ 0}$$

$$\mathbf{d}_2 = \mathbf{1\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 2}$$

$\langle \mathbf{d}_1, \mathbf{d2} \rangle = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$

$| \mathbf{d}_1 \| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{\mathbf{0.5}} = (42)^{\mathbf{0.5}} = 6.481$

$\| \mathbf{d}_2 \| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{\mathbf{0.5}} = (6)^{\mathbf{0.5}} = 2.449$

$\cos(\mathbf{d}_1, \mathbf{d}_2) = 0.3150$

Extended Jaccard Coefficient (Tanimoto)

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

$$EJ(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x} \cdot \mathbf{y}}{\|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 - \mathbf{x} \cdot \mathbf{y}}$$

Correlation measures the linear relationship between objects

$$\text{corr}(\mathbf{x},\mathbf{y}) = \frac{\text{covariance}(\mathbf{x},\mathbf{y})}{\text{standard\_deviation}(\mathbf{x}) * \text{standard\_deviation}(\mathbf{y})} = \frac{s_{xy}}{s_x\ s_y}, \quad (2.11)$$

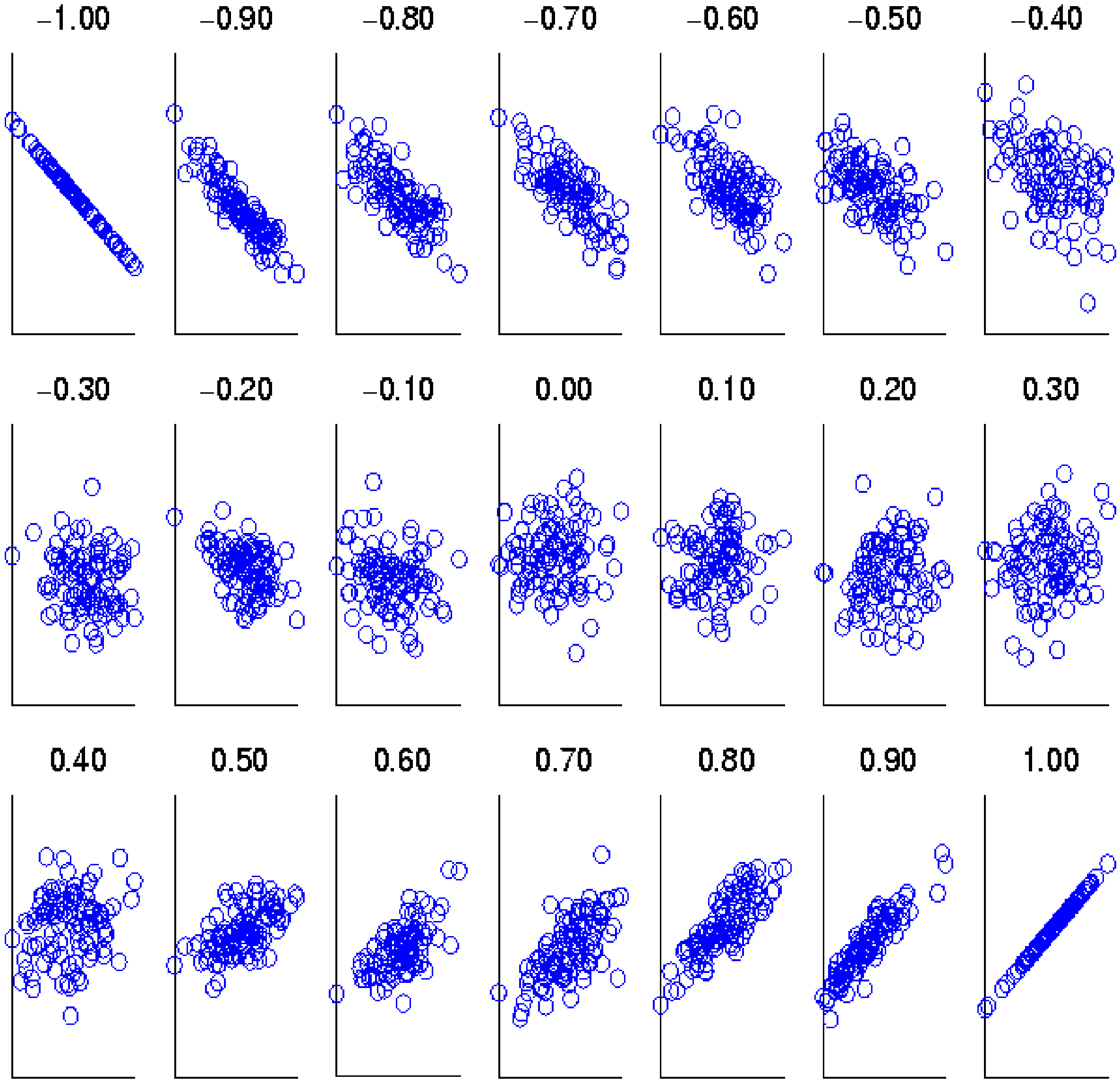
where we are using the following standard statistical notation and definitions

$$\text{covariance}(\mathbf{x},\mathbf{y}) = s_{xy} = \frac{1}{n-1}\sum_{k=1}^{n}(x_k - \overline{x})(y_k - \overline{y}) \qquad (2.12$$

$$\begin{aligned} \text{standard\_deviation}(\mathbf{x}) &= s_x = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(x_k - \overline{x})^2} \\ \text{standard\_deviation}(\mathbf{y}) &= s_y = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(y_k - \overline{y})^2} \end{aligned}$$

$$\begin{aligned} \overline{x} &= \frac{1}{n}\sum_{k=1}^{n} x_k \text{ is the mean of } \mathbf{x} \\ \overline{y} &= \frac{1}{n}\sum_{k=1}^{n} y_k \text{ is the mean of } \mathbf{y} \end{aligned}$$

Visually Evaluating Correlation



Scatter plots showing the similarity from –1 to 1.

Drawback of Correlation

- **x** = (-3, -2, -1, 0, 1, 2, 3)
- **y** = (9, 4, 1, 0, 1, 4, 9)

$y_{\mathrm{i}} = x_{\mathrm{i}}^2$

- mean(**x**) = 0, mean(**y**) = 4
- std(**x**) = 2.16, std(**y**) = 3.74

- corr = (-3)(5)+(-2)(0)+(-1)(-3)+(0)(-4)+(1)(-3)+(2)(0)+3(5) / (6 * 2.16 * 3.74)

  = 0

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, $s_k(\mathbf{x}, \mathbf{y})$, in the range [0, 1].

2: Define an indicator variable, δ_k, for the k^{th} attribute as follows:

δ_k = 0 if the k^{th} attribute is an asymmetric attribute and both objects have a value of 0, or if one of the objects has a missing value for the kth attribute

δ_k = 1 otherwise

3. Compute $\text{similarity}(\mathbf{x}, \mathbf{y}) = \dfrac{\sum_{k=1}^{n} \delta_k s_k(\mathbf{x}, \mathbf{y})}{\sum_{k=1}^{n} \delta_k}$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.
  - Use non-negative weights ω_k
  - $similarity(\mathbf{x},\mathbf{y}) = \frac{\sum_{k=1}^{n} \omega_k \delta_k s_k(\mathbf{x},\mathbf{y})}{\sum_{k=1}^{n} \omega_k \delta_k}$

- Can also define a weighted form of distance

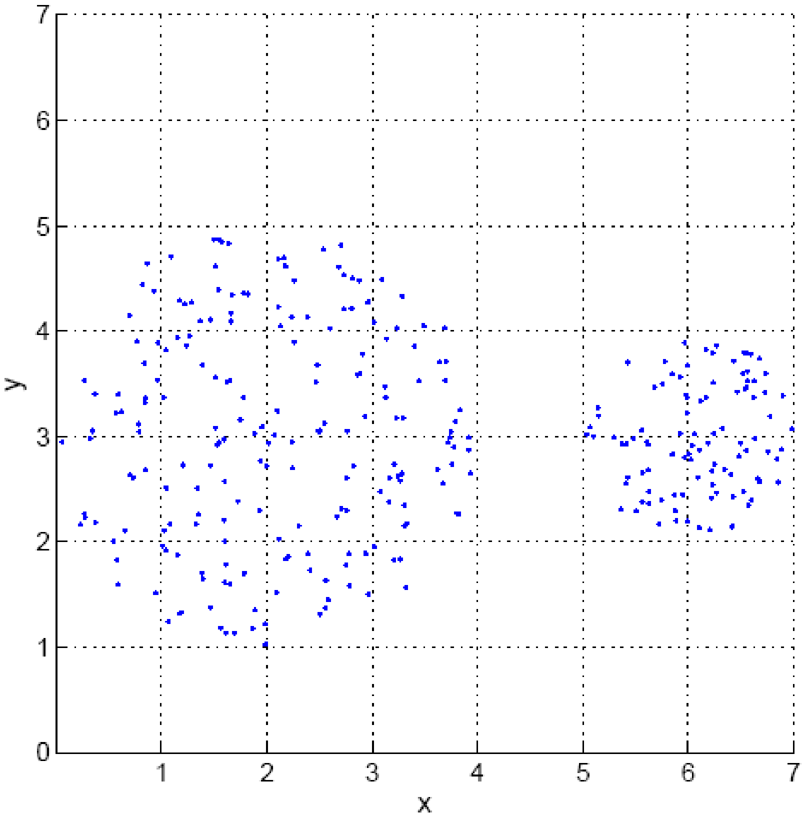
$$d(\mathbf{x},\mathbf{y}) = \left(\sum_{k=1}^{n} w_k |x_k - y_k|^r \right)^{1/r}$$

Density

- Measures the degree to which data objects are close to each other in a specified area
- The notion of density is closely related to that of proximity
- Concept of density is typically used for clustering and anomaly detection
- Examples:
  - Euclidean density
    - Euclidean density = number of points per unit volume
  - Probability density
    - Estimate what the distribution of the data looks like
  - Graph-based density
    - Connectivity

Euclidean Density: Grid-based Approach

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



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

Euclidean Density: Center-Based

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

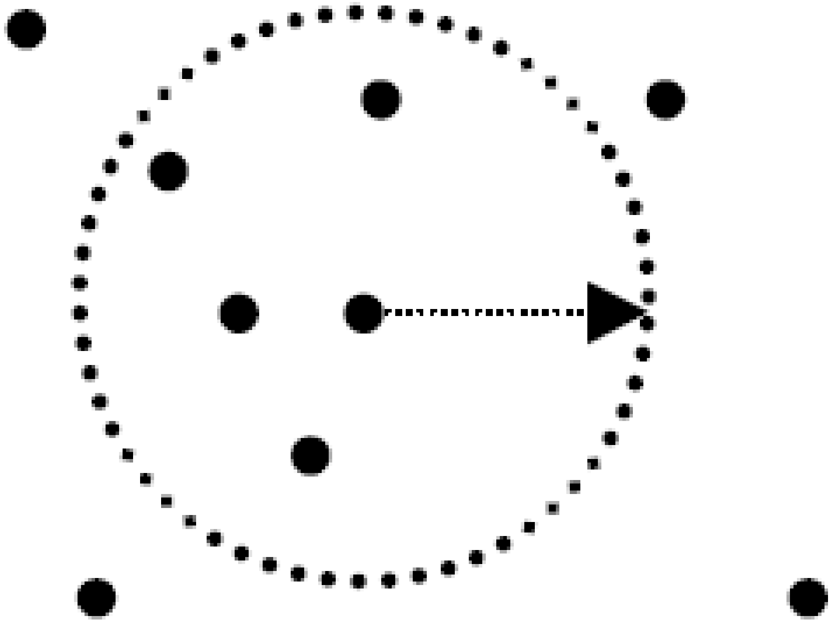


Illustration of center-based density.

Comparison of Proximity Measures

- Domain of application
  - Similarity measures tend to be specific to the type of attribute and data
  - Record data, images, graphs, sequences, 3D-protein structure, etc. tend to have different measures
- However, one can talk about various properties that you would like a proximity measure to have
  - Symmetry is a common one
  - Tolerance to noise and outliers is another
  - Ability to find more types of patterns?
  - Many others possible
- The measure must be applicable to the data and produce results that agree with domain knowledge

Information Based Measures

- Information theory is a well-developed and fundamental disciple with broad applications

- Some similarity measures are based on information theory
  - Mutual information in various versions
  - Maximal Information Coefficient (MIC) and related measures
  - General and can handle non-linear relationships
  - Can be complicated and time intensive to compute

Information and Probability

- Information relates to possible outcomes of an event
  - transmission of a message, flip of a coin, or measurement of a piece of data

- The more certain an outcome, the less information that it contains and vice-versa
  - For example, if a coin has two heads, then an outcome of heads provides no information
  - More quantitatively, the information is related the probability of an outcome
    - ◆ The smaller the probability of an outcome, the more information it provides and vice-versa
  - Entropy is the commonly used measure

Entropy

- For
  - a variable (event), X,
  - with n possible values (outcomes), x_1, x_2 ..., x_n
  - each outcome having probability, p_1, p_2 ..., p_n
  - the entropy of X , $H(X)$, is given by

$$H(X) = -\sum_{i=1}^{n} p_i \log_2 p_i$$

- Entropy is between 0 and $\log_2 n$ and is measured in bits
  - Thus, entropy is a measure of how many bits it takes to represent an observation of X on average

Entropy Examples

- For a coin with probability p of heads and probability $q = 1 – p$ of tails

$$H = -p \log_2 p - q \log_2 q$$

  - For p= 0.5, q = 0.5 (fair coin) $H = 1$
  - For $p = 1$ or $q = 1$, $H = 0$

- What is the entropy of a fair four-sided die?

Entropy for Sample Data: Example

Hair Color	Count	p	$-p\log_2 p$
Black	75	0.75	0.3113
Brown	15	0.15	0.4105
Blond	5	0.05	0.2161
Red	0	0.00	0
Other	5	0.05	0.2161
Total	100	1.0	1.1540

Maximum entropy is $\log_2 5 = 2.3219$

Entropy for Sample Data

- Suppose we have
  - a number of observations (m) of some attribute, X, e.g., the hair color of students in the class,
  - where there are n different possible values
  - And the number of observation in the i^{th} category is m_i
  - Then, for this sample

$$H(X) = -\sum_{i=1}^{n} \frac{m_i}{m} \log_2 \frac{m_i}{m}$$

- For continuous data, the calculation is harder

Mutual Information

- Information one variable provides about another

Formally, $I(X,Y) = H(X) + H(Y) - H(X,Y)$, where

$H(X,Y)$ is the joint entropy of X and Y,

$$H(X,Y) = -\sum_i \sum_j p_{ij} \log_2 p_{ij}$$

Where p_{ij} is the probability that the ith value of X and the jth value of Y occur together

- For discrete variables, this is easy to compute

- Maximum mutual information for discrete variables is $\log_2(\min(n_X, n_Y))$, where n_X (n_Y) is the number of values of X (Y)

Mutual Information Example

Student Status	Count	*p*	$-p\log_2 p$
Undergrad	45	0.45	0.5184
Grad	55	0.55	0.4744
Total	100	1.00	0.9928

Grade	Count	*p*	$-p\log_2 p$
A	35	0.35	0.5301
B	50	0.50	0.5000
C	15	0.15	0.4105
Total	100	1.00	1.4406

Student Status	Grade	Count	*p*	$-p\log_2 p$
Undergrad	A	5	0.05	0.2161
Undergrad	B	30	0.30	0.5211
Undergrad	C	10	0.10	0.3322
Grad	A	30	0.30	0.5211
Grad	B	20	0.20	0.4644
Grad	C	5	0.05	0.2161
Total		100	1.00	2.2710

Mutual information of Student Status and Grade = 0.9928 + 1.4406 - 2.2710 = 0.1624

Maximal Information Coefficient

- Reshef, David N., Yakir A. Reshef, Hilary K. Finucane, Sharon R. Grossman, Gilean McVean, Peter J. Turnbaugh, Eric S. Lander, Michael Mitzenmacher, and Pardis C. Sabeti. "Detecting novel associations in large data sets." *science* 334, no. 6062 (2011): 1518-1524.
- Applies mutual information to two continuous variables
- Consider the possible binnings of the variables into discrete categories
  - $n_X \times n_Y \leq N^{0.6}$ where
    - n_X is the number of values of X
    - n_Y is the number of values of Y
    - N is the number of samples (observations, data objects)
- Compute the mutual information
  - Normalized by $\log_2(\min(n_X, n_Y)$
- Take the highest value