Basic Concepts: Measuring Similarity between Objects

What Is Good Clustering?

- A good clustering method will produce high quality clusters which should have
  - **High intra-class similarity:** Cohesive within clusters
  - **Low inter-class similarity:** Distinctive between clusters
- **Quality function**
  - There is usually a separate "quality" function that measures the "goodness" of a cluster
  - It is hard to define "similar enough" or "good enough"
    - The answer is typically highly subjective
- There exist many similarity measures and/or functions for different applications
- Similarity measure is critical for cluster analysis

Similarity, Dissimilarity, and Proximity

- **Similarity measure** or **similarity function**
  - A real-valued function that quantifies the similarity between two objects
  - Measure how two data objects are alike: The higher value, the more alike
  - Often falls in the range [0,1]: 0: no similarity; 1: completely similar
- **Dissimilarity** (or **distance**) measure
  - Numerical measure of how different two data objects are
  - In some sense, the inverse of similarity: The lower, the more alike
  - Minimum dissimilarity is often 0 (i.e., completely similar)
  - Range [0, 1] or [0, ∞) , depending on the definition
- **Proximity** usually refers to either similarity or dissimilarity

Distance on Numeric Data: Minkowski Distance

Data Matrix and Dissimilarity Matrix

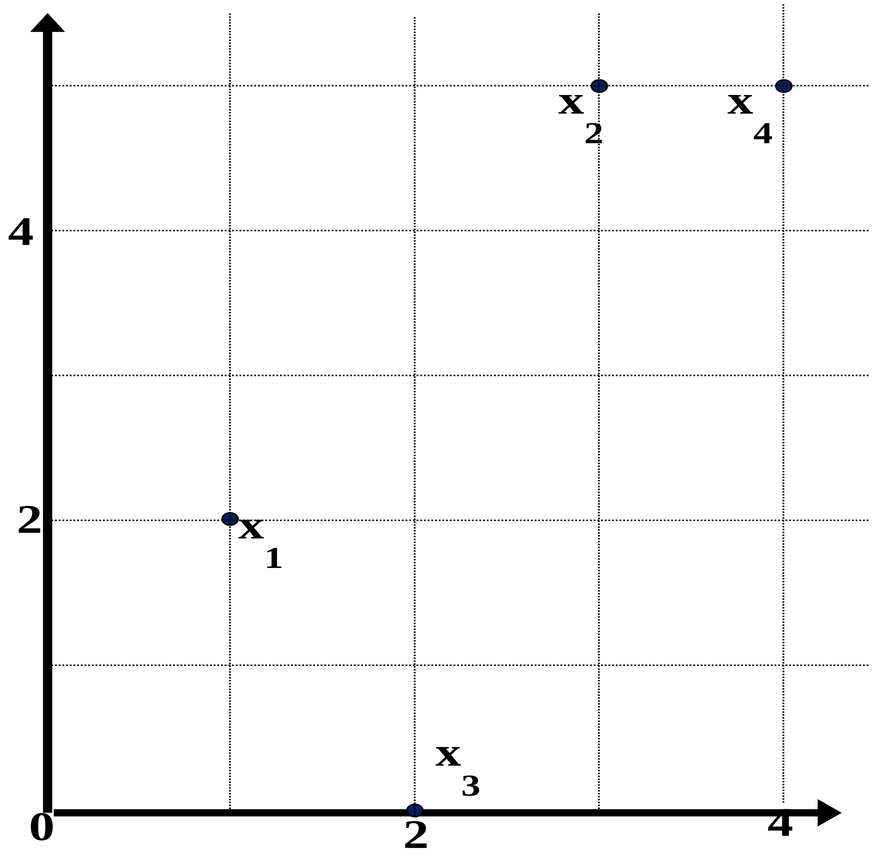
- Data matrix
  - A data matrix of n data points with *l* dimensions

$$D = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1l} \\ x_{21} & x_{22} & \dots & x_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nl} \end{pmatrix}$$

- Dissimilarity (distance) matrix
  - n data points, but registers only the distance *d*(*i, j*) (typically metric)
  - Usually symmetric, thus a triangular matrix
  - Distance functions are usually different for real, boolean, categorical, ordinal, ratio, and vector variables
  - Weights can be associated with different variables based on applications and data semantics

$$\begin{pmatrix} 0 & & & \\ d(2,1) & 0 & & \\ \vdots & \vdots & \ddots & \\ d(n,1) & d(n,2) & \dots & 0 \end{pmatrix}$$

Example: Data Matrix and Dissimilarity Matrix



Data Matrix

point	attribute1	attribute2
x1	1	2
x2	3	5
x3	2	0
x4	4	5

Dissimilarity Matrix (by Euclidean Distance)

	x1	*x2*	*x3*	*x4*
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Distance on Numeric Data: Minkowski Distance

- Minkowski distance: A popular distance measure

$$d(i, j) = \sqrt[p]{|x_{i1} - x_{j1}|^p + |x_{i2} - x_{j2}|^p + \cdots + |x_{il} - x_{jl}|^p}$$

where $i = (x_{i1}, x_{i2}, \ldots, x_{il})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jl})$ are two l-dimensional data objects, and p is the order (the distance so defined is also called L-p norm)

- Properties
  - d(i, j) > 0 if i ≠ j, and d(i, i) = 0 (Positivity)
  - d(i, j) = d(j, i) (Symmetry)
  - d(i, j) ≤ d(i, k) + d(k, j) (Triangle Inequality)
- A distance that satisfies these properties is a metric
- Note: There are nonmetric dissimilarities, e.g., set differences

Special Cases of Minkowski Distance

- p = 1: (L_1 norm) Manhattan (or city block) distance
  - E.g., the Hamming distance: the number of bits that are different between two binary vectors

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \cdots + |x_{il} - x_{jl}|$$

- p = 2: (L_2 norm) Euclidean distance

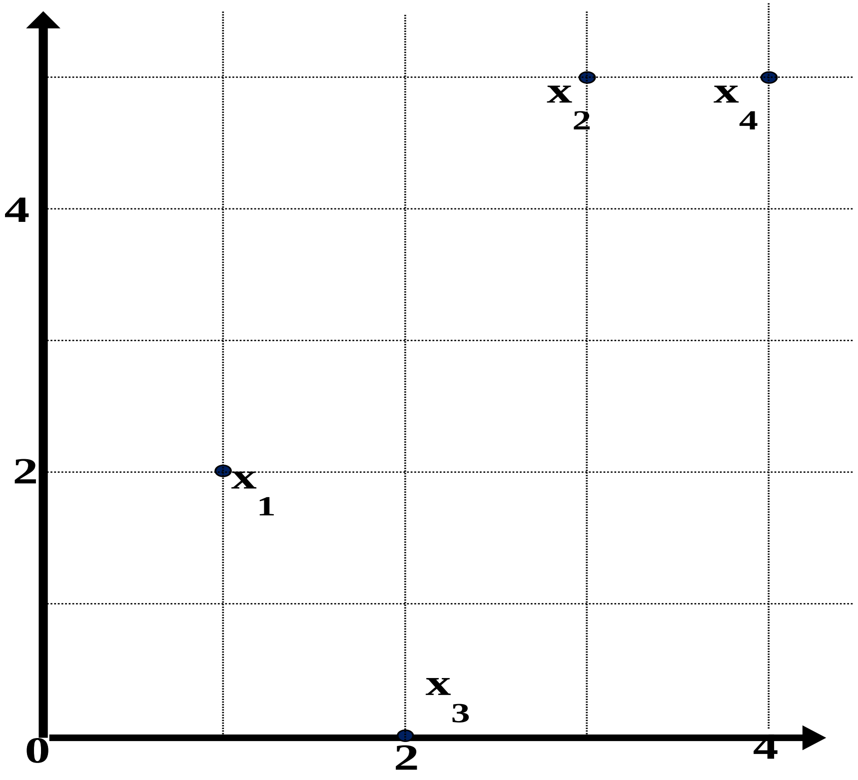
$$d(i, j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \cdots + |x_{il} - x_{jl}|^2}$$

- $p \to \infty$: (L_{max} norm, L_∞ norm) "supremum" distance
  - The maximum difference between any component (attribute) of the vectors

$$d(i, j) = \lim_{p \to \infty} \sqrt[p]{|x_{i1} - x_{j1}|^p + |x_{i2} - x_{j2}|^p + \cdots + |x_{il} - x_{jl}|^p} = \max_{f=1}^{l} |x_{if} - x_{jf}|$$

Example: Minkowski Distance at Special Cases

point	attribute 1	attribute 2
x1	1	2
x2	3	5
x3	2	0
x4	4	5



Manhattan (L_1)

L	x1	x2	x3	x4
x1	0			
x2	5	0		
x3	3	6	0	
x4	6	1	7	0

Euclidean (L_2)

L2	x1	x2	x3	x4
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Supremum (L_∞)

L_∞	x1	x2	x3	x4
x1	0			
x2	3	0		
x3	2	5	0	
x4	3	1	5	0

Proximity Measure for Symmetric vs. Asymmetric Binary Variables

Proximity Measure for Binary Attributes

- A contingency table for binary data

		Object j		
		1	0	sum
Object i	1	q	r	$q+r$
	0	s	t	$s+t$
	sum	$q+s$	$r+t$	p

- Distance measure for symmetric binary variables: $d(i,j) = \frac{r+s}{q+r+s+t}$
- Distance measure for asymmetric binary variables: $d(i,j) = \frac{r+s}{q+r+s}$
- Jaccard coefficient (*similarity* measure for *asymmetric* binary variables): $sim_{Jaccard}(i,j) = \frac{q}{q+r+s}$
- Note: Jaccard coefficient is the same as "coherence": (a concept discussed in Pattern Discovery)

$$coherence(i,j) = \frac{sup(i,j)}{sup(i) + sup(j) - sup(i,j)} = \frac{q}{(q+r) + (q+s) - q}$$

Example: Dissimilarity between Asymmetric Binary Variables

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N

Mary

Jack		1	0	Σ_{row}
	1	2	0	2
	0	1	3	4
	Σ_{col}	3	3	6

Jim

Jack		1	0	Σ_{row}
	1	1	1	2
	0	1	3	4
	Σ_{col}	2	4	6

Mary

Jim		1	0	Σ_{row}
	1	1	1	2
	0	2	2	4
	Σ_{col}	3	3	6

- Gender is a symmetric attribute (not counted in)
- The remaining attributes are asymmetric binary
- Let the values Y and P be 1, and the value N be 0
- Distance: $d(i, j) = \frac{r + s}{q + r + s}$

$$d(jack, mary) = \frac{0+1}{2+0+1} = 0.33$$

$$d(jack, jim) = \frac{1+1}{1+1+1} = 0.67$$

$$d(jim, mary) = \frac{1+2}{1+1+2} = 0.75$$

Distance between Categorical Attributes, Ordinal Attributes, and Mixed Types

Proximity Measure for Categorical Attributes

- Categorical data, also called nominal attributes
  - Example: Color (red, yellow, blue, green), profession, etc.
- Method 1: Simple matching
  - *m*: # of matches, *p*: total # of variables

$$d(i, j) = \frac{p - m}{p}$$

- Method 2: Use a large number of binary attributes
  - Creating a new binary attribute for each of the *M* nominal states

Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank (e.g., freshman, sophomore, junior, senior)
- Can be treated like interval-scaled
  - Replace *an ordinal variable value* by its rank: $r_{if} \in \{1, ..., M_f\}$
  - Map the range of each variable onto [0, 1] by replacing *i*-th object in the *f*-th variable by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

    - Example: freshman: 0; sophomore: 1/3; junior: 2/3; senior 1
      - Then distance: d(freshman, senior) = 1, d(junior, senior) = 1/3
  - Compute the dissimilarity using methods for interval-scaled variables

Attributes of Mixed Type

- A dataset may contain all attribute types
  - Nominal, symmetric binary, asymmetric binary, numeric, and ordinal
- One may use a weighted formula to combine their effects:

$$d(i, j) = \frac{\sum_{f=1}^{p} w_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^{p} w_{ij}^{(f)}}$$

  - If f is numeric: Use the normalized distance
  - If f is binary or nominal: $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$; or $d_{ij}^{(f)} = 1$ otherwise
  - If f is ordinal
    - Compute ranks z_{if} (where $z_{if} = \frac{r_{if} - 1}{M_f - 1}$)
    - Treat z_{if} as interval-scaled

Example

- Here we provide an example on how to calculate distance between categorical data points

- Given several attributes of a car and their values

	Attribute names	Possible values
1	Color	Black, Red, White
2	Make	Buick, Chevy, Dodge, Ford
3	Body Style	2-Door, 4-Door

- Given two cars:

	Color No	Make No	Body Style Yes
Car A	Red	Ford	4-Door
Car B	Black	Dodge	4-Door

- What is the distance between these cars, calculated by *simple match*?
- $d = \frac{m-p}{m} = \frac{3-1}{3} = \frac{2}{3}$
- m is the number of attributes; p is the number of exactly matched attributes

- Given several attributes of a car and their values

Attribute names	Possible values
Color	Black, Red, White
Make	Buick, Chevy, Dodge, Ford
Body Style	2-Door, 4-Door

- Given two cars:

	Color	Make	Body Style
Car A	Red	Ford	4-Door
Car B	Black	Dodge	4-Door

- Convert cars into a binary representations. Assuming attributes are symmetric. Calculate the distance.

- Given several attributes of a car and their values

Attribute names	Possible values
Color	Black, Red, White
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- Given two cars:

	Color	Make	Body Style
Car A	Red	Ford	4-Door
Car B	Black	Dodge	4-Door

- Convert cars into a binary representations.

	Color			Make				Body Style	
	B	R	W	BUIC	CHEV	DODG	FORD	2DR	4DR
Car A	0	1	0	0	0	0	1	0	1
Car B	1	0	0	0	0	1	0	0	1

- Given several attributes of a car and their values

Attribute names	Possible values
Color	Black, Red, White
Make	Buick, Chevy, Dodge, Ford
Body Style	2-Door, 4-Door

- Given two cars:

Car A	0	1	0	0	0	0	1	0	1
Car B	1	0	0	0	0	1	0	0	1

- Given several attributes of a car and their values

Attribute names	Possible values
Color	Black, Red, White
Make	Buick, Chevy, Dodge, Ford
Body Style	2-Door, 4-Door

- Given two cars:

Car A	0	1	0	0	0	0	1	0	1
Car B	1	0	0	0	0	1	0	0	1

- Assuming attributes are *symmetric*. Calculate the distance.
- $d = \frac{m-p}{m} = \frac{9-5}{9} = \frac{4}{9}$
- m is the number of attributes; p is the number of exactly matched attributes

- Given several attributes of a car and their values

Attribute names	Possible values
Color	Black, Red, White
Make	Buick, Chevy, Dodge, Ford
Body Style	2-Door, 4-Door

- Given two cars:

Car A	0	1	~~0~~	~~0~~	~~0~~	0	1	~~0~~	1
Car B	1	0	~~0~~	~~0~~	~~0~~	1	0	~~0~~	1

- Assuming attributes are *asymmetric*. Removing dimensions where both are 0! Calculate the distance.

- $d = \frac{m-p}{m} = \frac{5-1}{5} = \frac{4}{5}$

- m is the number of attributes; p is the number of exactly matched attributes

Proximity Measure between Two Vectors: Cosine Similarity

Cosine Similarity of Two Vectors

- A **document** can be represented by a bag of terms or a long vector, with each attribute recording the *frequency* of a particular term (such as word, keyword, or phrase) in the document

Document	team	coach	hockey	baseball	soccer	penalty	score	win	loss	season
Document1	5	0	3	0	2	0	0	2	0	0
Document2	3	0	2	0	1	1	0	1	0	1
Document3	0	7	0	2	1	0	0	3	0	0
Document4	0	1	0	0	1	2	2	0	3	0

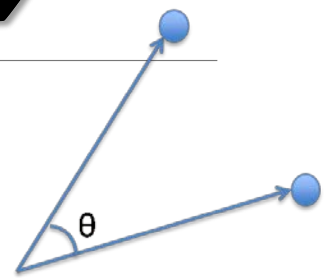
- Other vector objects: Gene features in micro-arrays
- Applications: Information retrieval, biologic taxonomy, gene feature mapping, etc.
- Cosine measure: If d_1 and d_2 are two vectors (e.g., term-frequency vectors), then

$$cos(d_1, d_2) = \frac{d_1 \bullet d_2}{\| d_1 \| \times \| d_2 \|}$$

where • indicates vector dot product, $||d||$: the length of vector d

Example: Calculating Cosine Similarity

- Calculating Cosine Similarity: $$cos(d_1, d_2) = \frac{d_1 \bullet d_2}{\| d_1 \| \times \| d_2 \|}$$ $$sim(A, B) = \cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$$



  where • indicates vector dot product, ||*d*||: the length of vector *d*

- Ex: Find the **similarity** between documents 1 and 2.

  d_1 = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0) d_2 = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1)

  - First, calculate vector dot product

    $d_1 \bullet d_2$ = 5 X 3 + 0 X 0 + 3 X 2 + 0 X 0 + 2 X 1 + 0 X 1 + 0 X 1 + 2 X 1 + 0 X 0 + 0 X 1 = 25

  - Then, calculate $||d_1||$ and $||d_2||$

$$\| d_1 \| = \sqrt{5\times5+0\times0+3\times3+0\times0+2\times2+0\times0+0\times0+2\times2+0\times0+0\times0} = 6.481$$

$$\| d_2 \| = \sqrt{3\times3+0\times0+2\times2+0\times0+1\times1+1\times1+0\times0+1\times1+0\times0+1\times1} = 4.12$$

  - Calculate cosine similarity: cos(d_1, d_2) = 26/ (6.481 X 4.12) = 0.94

Correlation Measures between Two Variables: Covariance and Correlation Coefficient

Variance for Single Variable

- The variance of a random variable *X* provides a measure of how much the value of *X* deviates from the mean or expected value of *X:*

$$\sigma^2 = \mathrm{var}(X) = E[(\mathrm{X}-\mu)^2] = \begin{cases} \sum_x (x-\mu)^2 f(x) & \text{if } X \text{ is discrete} \\ \int_{-\infty}^{\infty} (x-\mu)^2 f(x)dx & \text{if } X \text{ is continuous} \end{cases}$$

  - where σ^2 is the variance of X, σ is called *standard deviation*

    μ is the mean, and μ = E[X] is the expected value of X
  - That is, variance is the expected value of the square deviation from the mean
  - It can also be written as: $\sigma^2 = \mathrm{var}(X) = E[(\mathrm{X}-\mu)^2] = E[\mathrm{X}^2]-\mu^2 = E[\mathrm{X}^2]-[E(x)]^2$
- Sample variance is the average squared deviation of the data value x_i from the sample mean $\hat{\mu}$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\hat{\mu})^2$$

Covariance for Two Variables

- Covariance between two variables X_1 and X_2

$$\sigma_{12} = E[(X_1 - \mu_1)(X_2 - \mu_2)] = E[X_1 X_2] - \mu_1 \mu_2 = E[X_1 X_2] - E[X_1]E[X_2]$$

where $\mu_1 = E[X_1]$ is the respective mean or **expected value** of X_1; similarly for μ_2

- Sample covariance between X_1 and X_2: $\hat{\sigma}_{12} = \frac{1}{n}\sum_{i=1}^{n}(x_{i1} - \hat{\mu}_1)(x_{i2} - \hat{\mu}_2)$
- Sample covariance is a generalization of the sample variance:

$$\hat{\sigma}_{11} = \frac{1}{n}\sum_{i=1}^{n}(x_{i1} - \hat{\mu}_1)(x_{i1} - \hat{\mu}_1) = \frac{1}{n}\sum_{i=1}^{n}(x_{i1} - \hat{\mu}_1)^2 = \hat{\sigma}_1{}^2$$

- **Positive covariance:** If $\sigma_{12} > 0$
- **Negative covariance**: If $\sigma_{12} < 0$
- **Independence**: If X_1 and X_2 are independent, $\sigma_{12} = 0$ but the reverse is not true
  - Some pairs of random variables may have a covariance 0 but are not independent
  - Only under some additional assumptions (e.g., the data follow multivariate normal distributions) does a covariance of 0 imply independence

Example: Calculation of Covariance

- Suppose two stocks X_1 and X_2 have the following values in one week:
  - (2, 5), (3, 8), (5, 10), (4, 11), (6, 14)
- Question: If the stocks are affected by the same industry trends, will their prices rise or fall together?
- Covariance formula

$$\sigma_{12} = E[(X_1 - \mu_1)(X_2 - \mu_2)] = E[X_1 X_2] - \mu_1 \mu_2 = E[X_1 X_2] - E[X_1]E[X_2]$$

- Its computation can be simplified as: $\sigma_{12} = E[X_1 X_2] - E[X_1]E[X_2]$
  - $E(X_1) = (2 + 3 + 5 + 4 + 6)/ 5 = 20/5 = 4$
  - $E(X_2) = (5 + 8 + 10 + 11 + 14) /5 = 48/5 = 9.6$
  - $\sigma_{12} = (2\times5 + 3\times8 + 5\times10 + 4\times11 + 6\times14)/5 - 4 \times 9.6 = 4$
- Thus, X_1 and X_2 rise together since $\sigma_{12} > 0$

Correlation between Two Numerical Variables

- **Correlation** between two variables X_1 and X_2 is the standard covariance, obtained by normalizing the covariance with the standard deviation of each variable

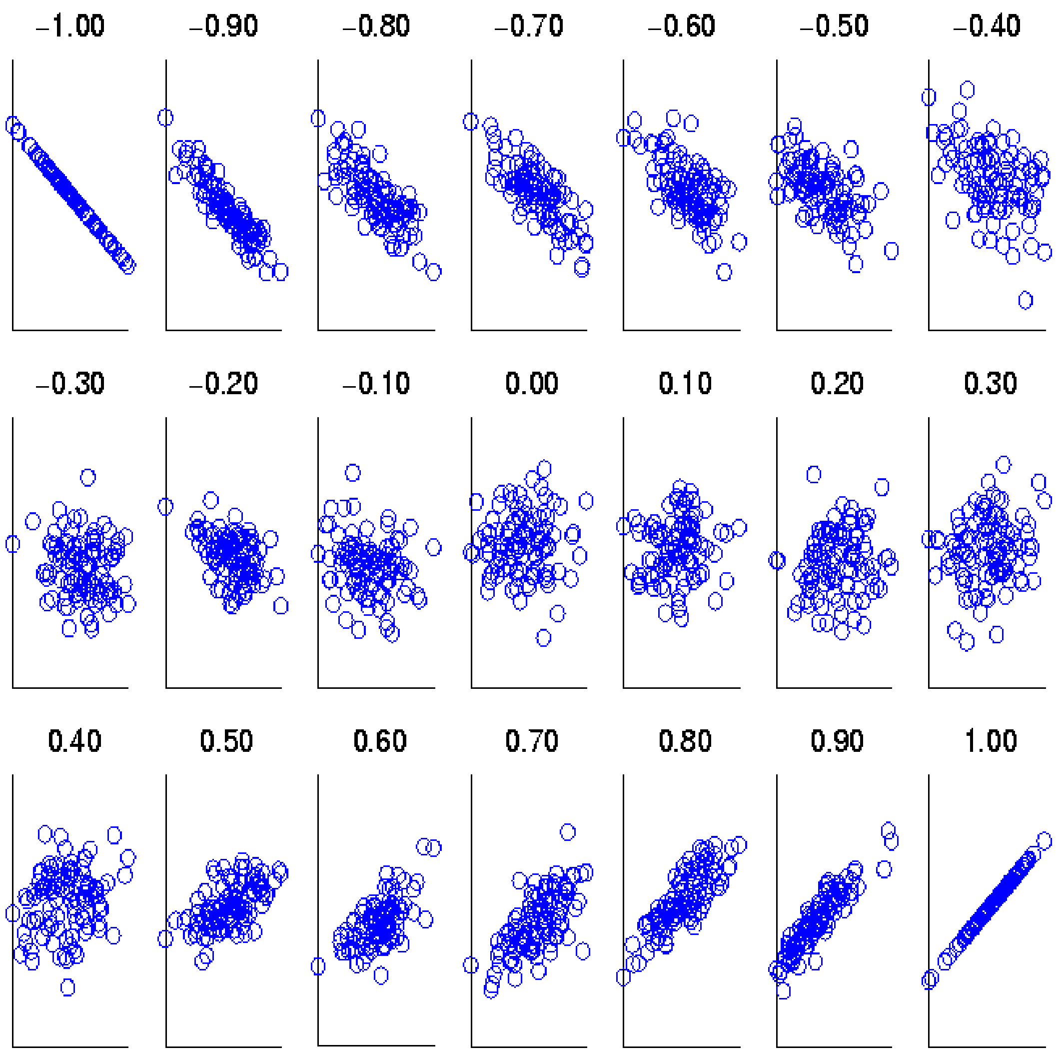
$$\rho_{12} = \frac{\sigma_{12}}{\sigma_1 \sigma_2} = \frac{\sigma_{12}}{\sqrt{\sigma_1{}^2 \sigma_2{}^2}}$$

- **Sample correlation** for two attributes X_1 and X_2: $\hat{\rho}_{12} = \frac{\hat{\sigma}_{12}}{\hat{\sigma}_1 \hat{\sigma}_2} = \frac{\sum_{i=1}^{n} (x_{i1} - \hat{\mu}_1)(x_{i2} - \hat{\mu}_2)}{\sqrt{\sum_{i=1}^{n} (x_{i1} - \hat{\mu}_1)^2 \sum_{i=1}^{n} (x_{i2} - \hat{\mu}_2)^2}}$

  where n is the number of tuples, μ_1 and μ_2 are the respective means of X_1 and X_2, σ_1 and σ_2 are the respective standard deviation of X_1 and X_2

- If $\rho_{12} > 0$: A and B are positively correlated (X_1's values increase as X_2's)
  - The higher, the stronger correlation
- If $\rho_{12} = 0$: independent (under the same assumption as discussed in co-variance)
- If $\rho_{12} < 0$: negatively correlated

Visualizing Changes of Correlation Coefficient



- Correlation coefficient value range: [–1, 1]
- A set of scatter plots shows sets of points and their correlation coefficients changing from –1 to 1

Covariance Matrix

- The variance and covariance information for the two variables X_1 and X_2 can be summarized as 2 X 2 covariance matrix as

$$\Sigma = E[(\mathbf{X}-\mu)(\mathbf{X}-\mu)^T] = E[(\begin{matrix} X_1-\mu_1 \\ X_2-\mu_2 \end{matrix})(X_1-\mu_1 \quad X_2-\mu_2)]$$

$$= \begin{pmatrix} E[(X_1-\mu_1)(X_1-\mu_1)] & E[(X_1-\mu_1)(X_2-\mu_2)] \\ E[(X_2-\mu_2)(X_1-\mu_1)] & E[(X_2-\mu_2)(X_2-\mu_2)] \end{pmatrix}$$

$$= \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{pmatrix}$$

- Generalizing it to *d* dimensions, we have,

$$D = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{d1} & x_{d2} & \cdots & x_{dd} \end{pmatrix} \quad \mathbf{\Sigma} = E[(\mathbf{X}-\mu)(\mathbf{X}-\mu)^T] = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{pmatrix}$$

Recommended Readings

- L. Kaufman and P. J. Rousseeuw, Finding Groups in Data: An Introduction to Cluster Analysis, John Wiley & Sons, 1990
- Mohammed J. Zaki and Wagner Meira, Jr.. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge University Press, 2014
- Jiawei Han, Micheline Kamber, and Jian Pei. Data Mining: Concepts and Techniques. Morgan Kaufmann, 3rd ed. , 2011
- Charu Aggarwal and Chandran K. Reddy (eds.). Data Clustering: Algorithms and Applications. CRC Press, 2014