

# Network structure identification

Network Application Diagnostics

B2M32DSA

Radek Mařík

Czech Technical University  
Faculty of Electrical Engineering  
Department of Telecommunication Engineering  
Prague CZ

October 24, 2017



## 1 Node Influence

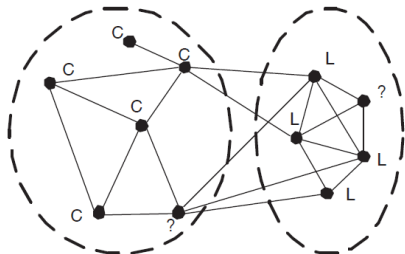
- Node Roles
- Hubs and Authorities

## 2 Network Clustering

- Multidimensional Clustering
- Clustering Coefficients
- Graph Laplacian



# Node Roles and Community Structure <sup>[STE07]</sup>



pre-dicting the political leaning of a person, either conservative (C) or liberal (L)

- *influence maximization* can be thought of as finding the best  $k$  people to target in order to maximize the number of people that will eventually be influenced
- *link-based classification* is the task of categorizing nodes using the node features and its link information



# Community Metric - Prerequisites <sup>[STE07]</sup>

- *Assumption*: a community is defined by a clique (maximal complete subgraph) in a network.
- **rawComm** is to be an approximate measure of the number of communities to which a node is attached.
- *incomplete edge* ... an edge that connects two nodes in different communities
- *impure edge* ... a non-link that appears within community.
- $p$  ... the probability that two linked nodes are in the same community

$$p = \frac{\text{Complete node pairs}}{\text{Total linked node pairs}}$$

- $q$  ... the probability that two non-linked nodes are in different communities.

$$q = \frac{\text{Pure node pairs}}{\text{Total non-linked node pairs}}$$



# Community Metric <sup>[STE07]</sup>

- **rawComm** metric

$$\text{rawComm} = \sum_{v \in N(u)} \tau_u(v)$$

where

- $N(u)$  ... the neighborhood of  $u$ ,  
that is all of the nodes that are directly linked to  $u$

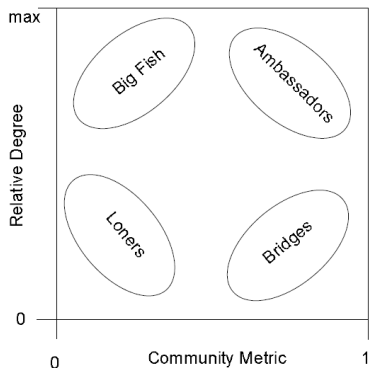
- 

$$\tau_u(v) = \frac{1}{1 + \sum_{v_j \in N(u)} I(v_i, v_j) \cdot p + \bar{I}(v_i, v_j) \cdot (1 - q)}$$

- $I(x, y)$  ... an indicator function that is 1 if there is a link between  $x$  and  $y$  and 0 otherwise.  $\bar{I}$  is 1 if there is not a link and 0 otherwise.
- The denominator in the definition of  $\tau$  is the expected number of other nodes in  $u$ 's neighborhood are in a community with  $v_i$ .
  - The 1 represents the node  $v_i$  itself.
  - $I(v_i, v_j) \cdot p + \bar{I}(v_i, v_j) \cdot (1 - q)$  ... the probability of  $v_i$  and  $v_j$  being in the same community.

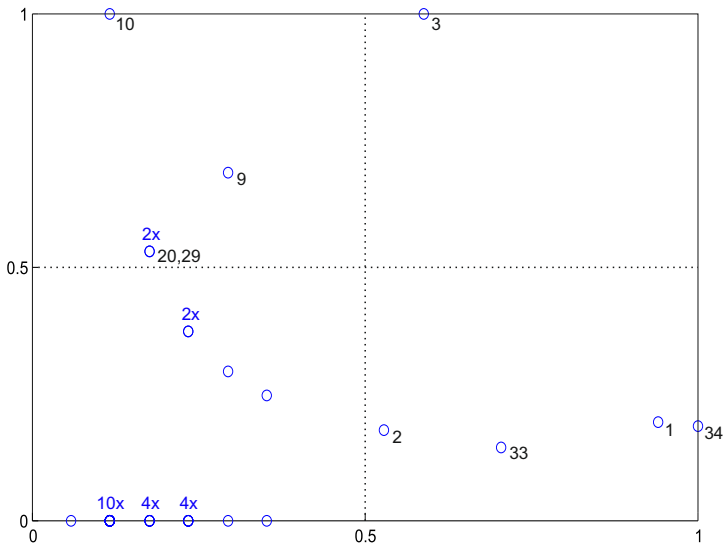


# Community-based Node Roles <sup>[STE07]</sup>

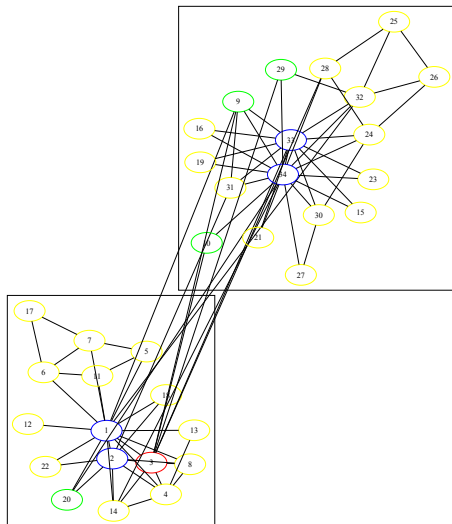


- a *authority* how much knowledge, information, etc. held by a node on a topic.
- a *hub* how well a node 'knows' where to find information on a given topic.
- an *ambassador* has links to many nodes from different communities
- a *big fish* has links only to other nodes in the same community
- a *bridge* because they serve as bridges between a small number of communities
- the *loners* . . . those with a low relative degree and low community

# Community-based Node Roles - Karate Club



# Community-based Node Roles - Karate Club





# Hubs and Authorities I [Kle98, Kle99, New10]

- Proposed by Kleinberg in 1998 [Kle98]
- In some networks it is appropriate also to accord a vertex high centrality if it points to others with high centrality
  - papers and their reviews
  - it makes sense only in directed networks (direction)
- **Authorities** are nodes that contain useful information on a topic of interest.
- **Hubs** are nodes that tell us where the best authorities are to be found.
- The centrality algorithm is called **hyperlink-induced topic search** or **HITS**
- Each vertex  $i$  has an authority centrality  $x_i$  and a hub centrality  $y_i$



# Hubs and Authorities II [Kle98, Kle99, New10]

- The authority centrality of a vertex is defined to be proportional to the sum of the hub centralities of the vertices that point to it:

$$x_i = \alpha \sum_j A_{ij} y_j$$

where  $\alpha$  is a constant.

- The hub centrality of a vertex is proportional to the sum of the authority centralities of the vertices it points to:

$$y_i = \beta \sum_j A_{ji} x_j$$

where  $\beta$  is a constant.

- In matrix terms

$$\mathbf{x} = \alpha \mathbf{A} \mathbf{y} \qquad \mathbf{y} = \beta \mathbf{A} \mathbf{x}$$

- Combining both and setting  $\gamma = (\alpha\beta)^{-1}$

$$\mathbf{A} \mathbf{A}^T \mathbf{x} = \gamma \mathbf{x} \qquad \mathbf{A}^T \mathbf{A} \mathbf{y} = \gamma \mathbf{y}$$



# Hubs and Authorities III

[Kle98, Kle99, New10]

$$\mathbf{A}\mathbf{A}^T \mathbf{x} = \gamma \mathbf{x}$$

$$\mathbf{A}^T \mathbf{A} \mathbf{y} = \gamma \mathbf{y}$$

- the authority and hub centralities are respectively given by eigenvectors of  $\mathbf{A}\mathbf{A}^T$  and  $\mathbf{A}^T \mathbf{A}$  with the same eigenvalue  $\gamma$ .
  - The same eigenvalue  $\gamma$ ?

$$\mathbf{A}\mathbf{A}^T \mathbf{x} = \gamma \mathbf{x} \quad \dots | \mathbf{A}^T \times \quad (1)$$

$$\mathbf{A}^T \mathbf{A} (\mathbf{A}^T \mathbf{x}) = \gamma (\mathbf{A}^T \mathbf{x}) \quad (2)$$

$$(3)$$

- The relation between both centralities

$$\mathbf{y} = \mathbf{A}^T \mathbf{x}$$

- $\mathbf{A}\mathbf{A}^T$  is the cocitation matrix.
- $\mathbf{A}^T \mathbf{A}$  is the bibliographic coupling matrix.
- HITS does not struggle with zero centralities outside strong components.



# Data Clustering [XW05, EK10]

- Data are **classified** or grouped into a set of categories or clusters.
  - **supervised** ... with a teacher
    - a finite set of class/category labels/tags is provided
  - **unsupervised** ... without a teacher
    - based on similarities of objects
- A **cluster** is a collection of objects that are similar to each other using some attribute.
- A cluster of objects can be treated as a group.
- Let  $P = \{p_1, \dots, p_N\}$  be a set of  $N$  data points representing  $N$  objects.
- The goal of **clustering** (CZ shlukování) is to divide  $P$  into  $K$  groups  $C_1, \dots, C_K$  so that data belonging to a group are more similar to each other than data from different groups.
- Each  $C_i$  is called a **cluster** (CZ shluk).
- Each object  $p_j$  is described by a vector  $\mathbf{x}_j = (x_{j1}, x_{j2}, \dots, x_{jd})^T \in \mathbb{R}^d$  and each measure  $x_{ji}$  is called to be a **feature** (attribute, dimension, or variable) (CZ příznak).



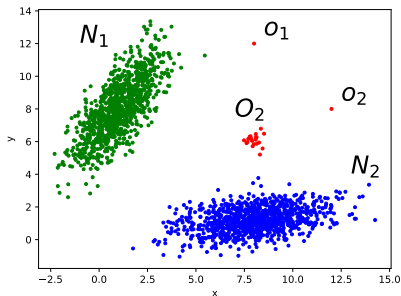
# Input Data <sup>[Agg17]</sup>

- Record data
  - Univariate
  - Multivariate
- Attributes
  - Binary/Boolean
  - Categorical
  - Continuous
  - Hybrid
- Relations
  - Sequential
    - Temporal
  - Spatial
  - Spatio-temporal
  - **Long range correlations**
  - **Graph**
- Data Quality
  - Data Fusion
  - Data Cleansing
  - Consistency maintenance
- Processing
  - Online/Offline processing
  - Distributed processing
  - **Analysis × Production**
    - Feature/Property searching/selection
    - Selected features detection
- Data Volume
  - Dense/**Sparse**
  - Low/High dimensions
  - Low/**Large volumes**
  - Big data
  - Internet of Things



# Simple Example - Multidimensional Space [CBK09]

- $N_1$  and  $N_2$  are regions of “normal” behavior
- Points  $o_1$  and  $o_2$  are anomalies
- Points in region  $O_3$  are anomalies



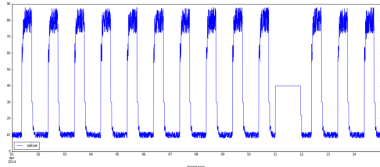
## Normal behavior

- **Normal distribution** ...  $N(\mu, \sigma)$ .  
Further, it will be referred as **Gaussian** distribution
- **Normal behavior/pattern** ... it is expected, not anomalous.

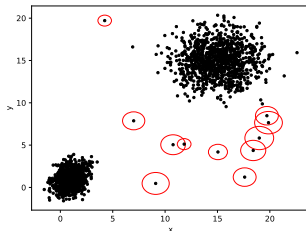


# Anomalies? Outliers?

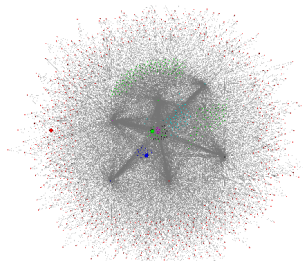
## Anomaly



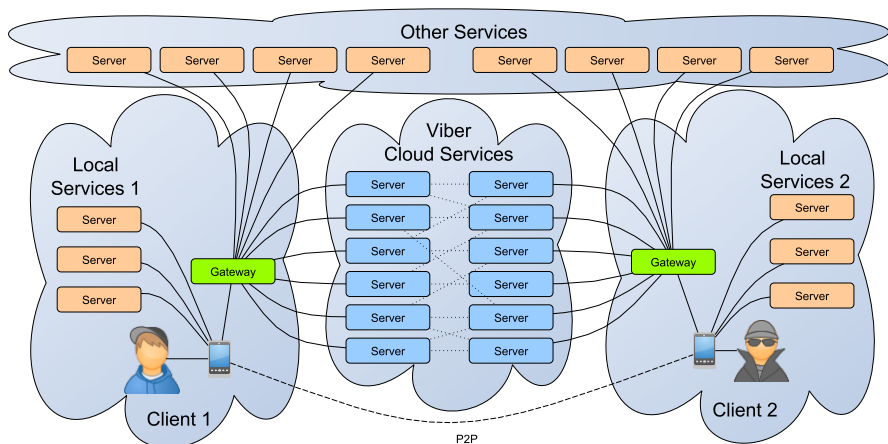
## Clouds of points (multi-dimensional)



## Complex Network

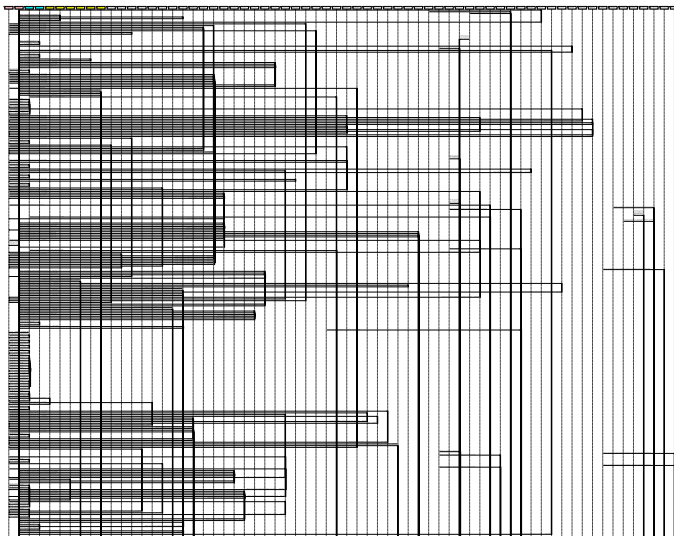


# Exemplar (Viber) Environment <sup>[MBKK15]</sup>





# Example Capture Characteristics - Message Sequences <sup>[MBKK15]</sup>

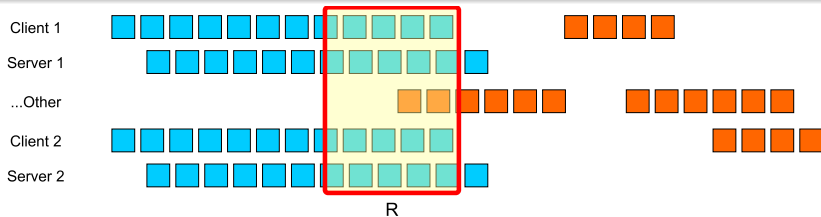


- 138882 PCAP blocks
- 1788 transport sessions
- 2 clients
- 22 viber.com servers
- 150 peers of 2 clients
- 5660 possible concurrent sessions
- **How to analyze?** 

# Concurrent Communication Detection <sup>[MBKK15]</sup>

## Selection of IP nodes

- *viber.com* servers → viber clients → other Viber servers
- Classified based on entropy based characteristics of TCP/IP distributions



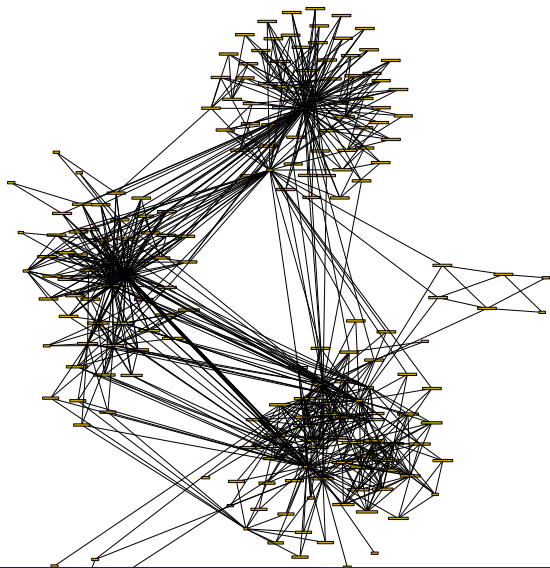
$$s(a, b) = \frac{\sum_{\forall i, j: t_a[i] - t_b[j] < R} R / (t_a[i] - t_b[j])}{\sum_{\forall i, j: t_a[i] - t_b[j] < R} 1}$$

In our experiments:  $R = 50ms$ ,  $s(a, b) > 0.001$



# UDP Packet Sequence Concurrency as a Complex Network

[MBKK15]



- Captures with two clients
- **Communities** of concurrent sessions
- Some clusters related to only one client
- Interesting clusters consist of nodes of **both** clients



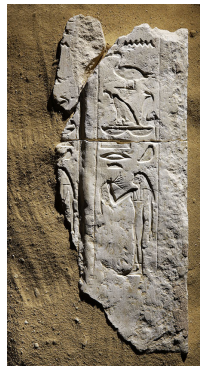
# Hierarchical or Partitional Clustering [XW05, EK10, eHS09]

- Partitional clustering** (CZ rozkladové shlukování)
  - the objects are divided into non-overlapping, unnested, clusters
  - Given a set of input patterns  $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$
  - It attempts to seek a  $K$ -partition of  $\mathbf{X}$ ,  $C = \{C_1, \dots, C_K\}$ , ( $K \leq N$ ) so that
    - $C_i \neq \emptyset, i = 1, \dots, K;$
    - $\bigcup_{i=1}^K C_i = \mathbf{X};$
    - $C_i \cap C_j = \emptyset; i, j = 1, \dots, K$  and  $i \neq j.$
- Hierarchical clustering** (CZ hierarchické shlukování)
  - the clusters are nested and can be displayed as a tree
  - It attempts to construct a tree-like nested structure partition of  $\mathbf{X}$ ,  $H = \{H_1, \dots, H_Q\}$ , ( $Q \leq N$ ) so that
 
$$C_i \in H_m, C_j \in H_\ell, \text{ and } m > \ell \implies C_i \subset C_j \text{ or } C_i \cap C_j = \emptyset \quad (4)$$

$$\text{for all } i, j \neq i, m, l = 1, \dots, Q \quad (5)$$
- The tree-like partition can visualizes as a **dendrogram**



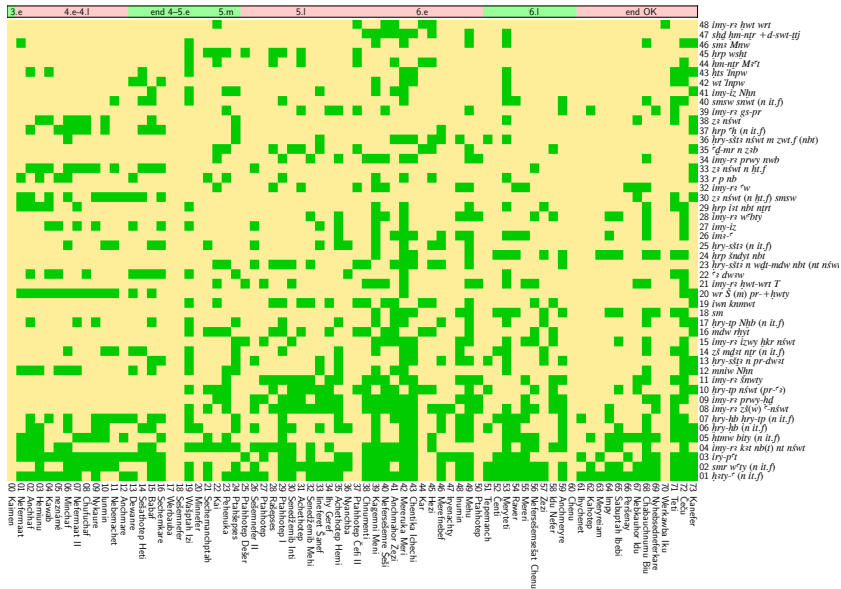
# Input Data - The Old Kingdom of Egypt <sup>[MD15]</sup>



- Continuous ... tomb dimensions
- Categorical ... titles
- Binary, boolean ... titles
- Multivariate ... people, titles, tombs
- Temporal ... dynasties, king reigns
- Spatio-temporal ... location of tombs in time

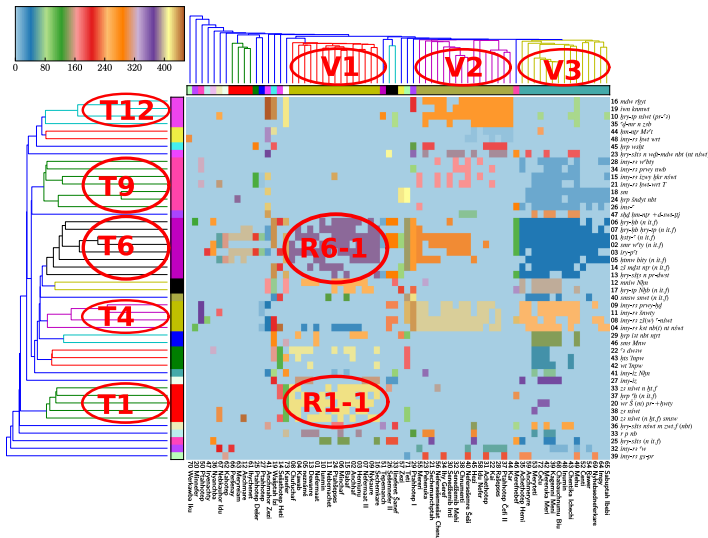


## Titles of Viziers [DMBC17]



# Titles of Viziers - Jaccard, Single Linkage Clustering

[DMBC17, JD88]



# Clustering <sup>[XW05, EK10]</sup>

- The steps of **cluster analysis**:
  - ① **Feature selection and extraction** selects distinguishing features from a set of candidates.
  - ② **Clustering algorithm design or selection** in which a proximity measure, a criterion function and an algorithm is determined.
  - ③ **Cluster validation** is performed to provide the users with a degree of confidence that the clustering results make sense.
  - ④ **Results interpretation** in which experts in the relevant fields interpret the data partition.
- The assigned **membership** of the nodes in the resulting clusters:
  - **Disjoint clusters** ... each node is a member of exactly one cluster.
  - **Overlapping clusters** ... a node may be a member of more than one cluster.
  - **Fuzzy clustering** methods assign a membership weight between 0 and 1 to each node such that  
1 means absolute membership,  
0 means a non-member.





# K-Means Clustering

[For65, Mac67, Har75, HW79, Llo06, XW05, EK10]

- Proposed by Lloyd in 1957 and published in 1982 <sup>[Llo06]</sup> and by Forgy in 1965 <sup>[For65]</sup>
- The term “k-means” was first used by MacQueen in 1967 <sup>[Mac67]</sup>
- A partitional clustering
- Given a set of observations  $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$
- The aim to minimize the within-cluster sum of squares (WCSS)

$$WCSS = \operatorname{argmin}_C \sum_{i=1}^K |C_i| \operatorname{Var}(C_i) = \operatorname{argmin}_C \sum_{i=1}^K \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2$$

- The mean  $\boldsymbol{\mu}_i$  of the data points within the cluster  $C_i$ :

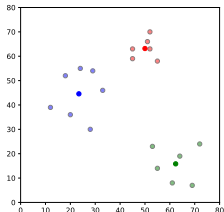
$$\boldsymbol{\mu}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in C_i} \mathbf{x}$$



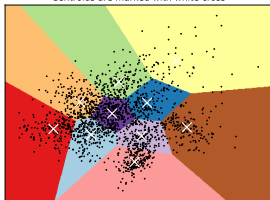
# K-Means Algorithm [HW79, EK10]

## $K$ -means Algorithm Basic Structure

- 1: **Input:**  $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$
- 2: **Input:**  $K$  ▷ a given number of clusters
- 3: **Output:**  $K$  clusters
- 4: **select**  $K$  points as the initial centroids
- 5: **repeat**
- 6:     **assign** each data point to its closest centroid and form clusters
- 7:     **compute** the centroid for each cluster
- 8: **until** centroids do not change significantly



K-means clustering on the digits dataset (PCA-reduced data)  
Centroids are marked with white cross



[PVG<sup>+</sup>11]



# Summary of Approaches [New06, Weh13, CRTV07, HK13]

- The **density** of graph is the proportion of present lines to the maximum possible number of lines.
- **Clustering coefficient** is a measure of the degree to which nodes in a graph tend to cluster together

## Global clustering coefficient [HK13]

the ratio of the total number of triangles to the total number of connected triplets.

$$C_g = \frac{2 \sum_{i=1}^N \ell_i}{\sum_{i=1}^N d_i(d_i - 1)}$$

- **Modularity** ... is - up to a normalization constant - the number of edges within communities  $c$  minus those for a **null model**
  - *"A good division of a network into communities is not merely one in which there are few edges between communities; it is one in which there are fewer than expected edges between communities".*



# Clustering, Triplets and Triangles [CRTV07, HK13]

## Clustering coefficient

- a measure of the degree to which nodes in a graph tend to cluster together
- a group of nodes with a relatively high density of ties
- $\ell_i$  ... the number of edges between neighbors of  $v_i$

## A triplet

- **open triangle** ... three nodes connected by two undirected ties
- of nodes  $(v_j, v_i, v_k)$  is called **connected** if  $v_j$  is connected to  $v_i$ ,  $v_i$  is connected to  $v_k$ , and  $j < k$ . Formally, if  $A_{ji} = 1$ ,  $A_{ik} = 1$ , and  $j < k$ .

## A triangle

- **closed triangle** ... a triplet connected by three undirected ties
- is a connected triplet  $(v_j, v_i, v_k)$  in which  $v_j$  and  $v_k$  are connected. Formally, if  $A_{jk} = 1$ .

# Numbers of Triplets and Triangles [CRTV07, HK13]

For a specific node  $v_i$

- a triplet ... if  $j < k$  and  $A_{ji}A_{ik} = 1$
- a triangle ... if  $j < k$  and  $A_{ji}A_{ik}A_{jk} = 1$
- a number of connected triplets

$$N_3(i) = \sum_{j < k} A_{ji}A_{ik} = d_i(d_i - 1)/2$$

- a number of choices how edges incident to  $v_i$  can be combined.
- a number triangles

$$N_{\Delta}(i) = \sum_{j < k} A_{ji}A_{ik}A_{jk}$$

- the number of edges between neighbors of  $v_i$

# Clustering coefficient <sup>[CRTV07, HK13]</sup>

Transitivity, Transitivity Ratio <sup>[CRTV07]</sup>

$$C = \frac{3N_{\Delta}}{N_3}$$

Clustering Coefficient, Local Clustering Coefficient <sup>[CRTV07, HK13]</sup>

$$C_i = \frac{N_{\Delta}(i)}{N_3(i)} = \frac{2\ell_i}{d_i(d_i - 1)}$$

Network average clustering coefficient <sup>[HK13]</sup>

$$C_{\ell} = 1/n \sum_{i=1}^N C_i$$

Global clustering coefficient <sup>[HK13]</sup>

the ratio of the total number of triangles to the total number of connected triplets.

$$C_g = \frac{2 \sum_{i=1}^N \ell_i}{\sum_{i=1}^N d_i(d_i - 1)}$$



# Diffusion Equation <sup>[Cra75]</sup>

- The **diffusion equation** is a partial differential equation.
- In physics, it describes the behavior of the *collective motion* of micro-*particles* in a material resulting from the random movement of each micro-particle.

$$\frac{\partial \phi(\mathbf{r}, t)}{\partial t} = \nabla \cdot [D(\phi, \mathbf{r}) \nabla \phi(\mathbf{r}, t)]$$

- where  $\phi(\mathbf{r}, t)$  is the density of the diffusing material
- at location  $\mathbf{r}$  and time  $t$  and
- $D(\phi, \mathbf{r})$  is the collective diffusion coefficient for density  $\phi$  at location  $\mathbf{r}$ ; and
- $\nabla$  represent the vector differential operator del (nabla).
- If  $D$  is constant, then the equation reduces to the linear differential equation (the **heat equation**),  $\nabla^2$  is the Laplacian operator:

$$\frac{\partial \phi(\mathbf{r}, t)}{\partial t} = D \nabla^2 \phi(\mathbf{r}, t) \quad \Delta = \nabla^2 = \sum_{k=1}^n \frac{\partial^2}{\partial x_k^2}$$



# Diffusion on Networks <sup>[New10]</sup>

- **Diffusion process** as a simple model of spread across a network
  - the spread of an idea,
  - the spread of a disease/virus
- An amount  $\psi_i$  of some commodity or substance at vertex  $i$ .
- The commodity flows from vertex  $i$  to an adjacent one  $j$  at a rate  $C(\psi_j - \psi_i)$
- where  $C$  is a constant called the **diffusion constant**.
- The rate at which  $\psi_i$  is changing is given by

$$\frac{d\psi_i}{dt} = C \sum_j A_{ij}(\psi_j - \psi_i)$$

- The equation works for both undirected and directed networks.
- Let us assume an undirected and simple network.





# Diffusion Matrix Form Derivation <sup>[New10]</sup>

- Network diffusion equation

$$\frac{d\psi_i}{dt} = C \sum_j A_{ij} (\psi_j - \psi_i)$$

- Splitting, rewriting, merging

$$\begin{aligned} \frac{d\psi_i}{dt} &= C \sum_j A_{ij} \psi_j - C \psi_i \sum_j A_{ij} \\ &= C \sum_j A_{ij} \psi_j - C \psi_i k_i \\ &= C \sum_j (A_{ij} - \delta_{ij} k_i) \psi_j \end{aligned}$$

- where  $k_i = \sum_j A_{ij}$  is the degree of vertex  $i$  and
- $\delta_{ij}$  is the Kronecker delta.



# Diffusion Matrix Form <sup>[New10]</sup>

- Network diffusion equation

$$\frac{d\psi_i}{dt} = C \sum_j (A_{ij} - \delta_{ij}k_i)\psi_j$$

- In matrix form

$$\frac{d\psi}{dt} = C(\mathbf{A} - \mathbf{D})\psi$$

- where  $\psi$  is the vector whose components are amounts  $\psi_i$ ,
- $\mathbf{A}$  is the adjacency matrix, and
- $\mathbf{D}$  is the diagonal matrix with the vertex degrees along the diagonal

$$\mathbf{D} = \begin{pmatrix} k_1 & 0 & 0 & \dots \\ 0 & k_2 & 0 & \dots \\ 0 & 0 & k_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



# Graph Laplacian [New10, EK10]

- Network diffusion equation

$$\frac{d\psi}{dt} = C(\mathbf{A} - \mathbf{D})\psi$$

- In matrix form
- where  $\psi$  is the vector whose components are amounts  $\psi_i$ ,
- $\mathbf{A}$  is the adjacency matrix, and
- The **graph Laplacian** is the real symmetric matrix

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

$$L_{ij} = \begin{cases} k_i & \text{if } i = j, \\ -1 & \text{if } i \neq j \text{ and there is an edge between vertices } j \text{ and } i, \\ 0 & \text{otherwise} \end{cases}$$

$$L_{ij} = \delta_{ij}k_i - A_{ij}$$



# Diffusion Equation Solution <sup>[New10]</sup>

- Network diffusion equation

$$\frac{d\psi}{dt} = C(\mathbf{A} - \mathbf{D})\psi \quad \Rightarrow \quad \frac{d\psi}{dt} = -C\mathbf{L}\psi$$

- Assuming the vector  $\psi$  as a linear combination of the Laplacian eigenvectors  $\mathbf{v}_i$ , i.e.  $\mathbf{L}\mathbf{v}_i = \lambda_i\mathbf{v}_i$  and  $\mathbf{v}_i \cdot \mathbf{v}_j = 0$  for  $i \neq j$  (real, sym  $\mathbf{L}$ )

$$\psi(t) = \sum_i a_i(t)\mathbf{v}_i$$

- with the coefficients  $a_i(t)$  varying over time.
- By the substitution into the diffusion equation and the dot product with  $\mathbf{v}_j$

$$\sum_i \left( \frac{da_i}{dt} + C\lambda_i a_i \right) \mathbf{v}_i = 0 \quad \xrightarrow{\cdot \mathbf{v}_j} \quad \frac{da_i}{dt} + C\lambda_i a_i = 0$$

- The solution

$$a_i(t) = a_i(0)e^{-C\lambda_i t}$$



# Eigenvalues of the Graph Laplacian <sup>[New10]</sup>

- Let  $\mathbf{B}$  be the edge incidence matrix (i.e. edges  $\times$  vertices)
  - If  $i \neq j$  then  $\sum_k B_{ki}B_{kj}$  is  $-1$  if there is an edge between vertices  $i$  and  $j$ , and zero otherwise.
  - If  $i = j$  then  $\sum_k B_{ki}^2$  has a term  $+1$  for every edge connected to vertex  $i$  so that the sum is equal to the degree  $k_i$  of vertex  $i$ .

$$L_{ij} = \sum_k B_{ki}B_{kj} \quad \Rightarrow \quad \mathbf{L} = \mathbf{B}^T\mathbf{B}$$

- Let  $\mathbf{v}_i$  be an eigenvector of  $\mathbf{L}$  with eigenvalue  $\lambda_i$ , i.e.  $\mathbf{L}\mathbf{v}_i = \lambda_i\mathbf{v}_i$ .

$$\mathbf{v}_i^T \mathbf{B}^T \mathbf{B} \mathbf{v}_i = \mathbf{v}_i^T \mathbf{L} \mathbf{v}_i = \lambda_i \mathbf{v}_i^T \mathbf{v}_i = \lambda_i \quad \text{as } \mathbf{v}_i^T \mathbf{v}_i = 1$$

- It is just an inner product of a real vector ( $\mathbf{B}\mathbf{v}_i$ ) with itself.
  - $\Rightarrow$  It is a sum of squares  $\Rightarrow$  the sum  $\geq 0 \Rightarrow \lambda_i \geq 0$ .
  - The solution of the diff. equation contains only decaying exponentials.
  - The solution tends to an equilibrium value as  $t \rightarrow \infty$ .
- $\mathbf{L} \cdot \mathbf{1} = \mathbf{0} \Leftrightarrow \sum_j L_{ij} \times 1 = \sum_j (\delta_{ij}k_i - A_{ij}) = k_i - \sum_j A_{ij} = k_i - k_i = 0$ 
  - $\mathbf{1}$  is always an eigenvector of  $\mathbf{L}$  with the smallest eigenvalue  $\lambda_1 = 0$
  - $\Rightarrow \mathbf{L}$  is singular, the Laplacian has no inverse.



# Eigenvalues of the Graph Laplacian <sup>[New10]</sup>

- Let  $\mathbf{B}$  be the edge incidence matrix (i.e. edges  $\times$  vertices)
  - If  $i \neq j$  then  $\sum_k B_{ki}B_{kj}$  is  $-1$  if there is an edge between vertices  $i$  and  $j$ , and zero otherwise.
  - If  $i = j$  then  $\sum_k B_{ki}^2$  has a term  $+1$  for every edge connected to vertex  $i$  so that the sum is equal to the degree  $k_i$  of vertex  $i$ .

$$L_{ij} = \sum_k B_{ki}B_{kj} \quad \Rightarrow \quad \mathbf{L} = \mathbf{B}^T\mathbf{B}$$

- Let  $\mathbf{v}_i$  be an eigenvector of  $\mathbf{L}$  with eigenvalue  $\lambda_i$ , i.e.  $\mathbf{L}\mathbf{v}_i = \lambda_i\mathbf{v}_i$ .

$$\mathbf{v}_i^T \mathbf{B}^T \mathbf{B} \mathbf{v}_i = \mathbf{v}_i^T \mathbf{L} \mathbf{v}_i = \lambda_i \mathbf{v}_i^T \mathbf{v}_i = \lambda_i \quad \text{as } \mathbf{v}_i^T \mathbf{v}_i = 1$$

- It is just an inner product of a real vector ( $\mathbf{B}\mathbf{v}_i$ ) with itself.
  - $\Rightarrow$  It is a sum of squares  $\Rightarrow$  the sum  $\geq 0 \Rightarrow \lambda_i \geq 0$ .
  - The solution of the diff. equation contains only decaying exponentials.
  - The solution tends to an equilibrium value as  $t \rightarrow \infty$ .
- $\mathbf{L} \cdot \mathbf{1} = \mathbf{0} \Leftrightarrow \sum_j L_{ij} \times 1 = \sum_j (\delta_{ij}k_i - A_{ij}) = k_i - \sum_j A_{ij} = k_i - k_i = 0$ 
  - $\mathbf{1}$  is always an eigenvector of  $\mathbf{L}$  with the smallest eigenvalue  $\lambda_1 = 0$
  - $\Rightarrow \mathbf{L}$  is singular, the Laplacian has no inverse.



# Algebraic Connectivity <sup>[New10]</sup>

$$\mathbf{L} = \left( \begin{array}{cc|cc|cc|c} & & & & & & & \\ & L_1 & & & & & & \\ & & & & & & & \\ 0 & 0 & & & & & & \\ 0 & 0 & L_2 & & & & & \\ 0 & 0 & & & & & & \\ 0 & 0 & 0 & 0 & & & \ddots & \\ 0 & 0 & 0 & 0 & & & & \end{array} \right)$$

$$\mathbf{v} = (\underbrace{1, 1, 1, \dots}_{n_1 \text{ ones}}, \underbrace{0, 0, 0, \dots}_{\text{zeros}})$$

- Suppose we have a network that is divided up into  $c$  different components of sizes  $n_1, n_2, \dots, n_c$ .
- $\implies$  at least  $c$  eigenvectors with eigenvalue zero
- The number of zero eigenvalues is always exactly equal to the number of components.
- The second eigenvalue  $\lambda_2$  is non-zero if and only if the network is connected, it is called the **algebraic connectivity**.



# Summary

- Node roles
- Hubs and Authorities (HITS)
- Data Clustering
  - Introduction and examples
  - K-means clustering
- Clustering, triplets, and triangles
- Diffusion Equation
  - Graph Laplacian





# Competencies

- What are the basic roles of nodes?
- How is it possible to assess a role of a given nodes?
- Provide definitions of authorities and hubs.
- How are the hub and authority centralities defined?
- What is the goal of clustering?
- What are the two fundamental approaches to data clustering?
- What are the typical steps of a cluster analysis?
- What are the basic forms of node memberships in clusters?
- Describe k-means clustering.
- Define a triplet and triangle.
- Describe a diffusion equation.
- What is the graph Laplacian?
- Name basic properties of the graph Laplacian eigenvalues?



# References I

- [Agg17] Charu C. Aggarwal. *Outlier Analysis*. Springer, second edition, 2017.
- [CBK09] Varun Chandola, Arindam Banerjee, and Vipin Kumar. Anomaly detection: A survey. *ACM Comput. Surv.*, 41(3):15:1–15:58, July 2009.
- [Cra75] J. Crank. *The mathematics of diffusion*. Clarendon Press, second edition, 1975.
- [CRTV07] L. D. F. Costa, F. A. Rodrigues, G. Travieso, and P. R. Villas Boas. Characterization of complex networks: A survey of measurements. *Advances in Physics*, 56:167–242, January 2007.
- [DMBC17] Veronika Dulíková, Radek Mařík, Miroslav Barta, and Matej Cibulá. HMM model vývoje a trendů správy země v období Staré říše. In *16. ročník konference Počítačová podpora v archeologii, Písek CZ, 29. - 31. května 2017*. Katedra archeologie Západočeské univerzity v Plzni, CZ, 2017.
- [eHS09] Hana Řezanková, Dušan Húsek, and Václav Snášel. *Shluková analýza dat*. Professional Publishing, Praha, second edition, 2009.
- [EK10] David Easley and Jon Kleinberg. *Networks, Crowds, and Markets. Reasoning About a Highly Connected World*. Cambridge University Press, July 2010.
- [For65] E. Forgy. Cluster analysis of multivariate data: Efficiency versus interpretability of classification. *Biometrics*, 21(3):768–769, 1965.
- [Har75] J.A. Hartigan. *Clustering Algorithms*. John Wiley & Sons Inc., New York, 1975.
- [HK13] Stephen J. Hardiman and Liran Katzir. Estimating clustering coefficients and size of social networks via random walk. In *Proceedings of the 22Nd International Conference on World Wide Web, WWW '13*, pages 539–550, Republic and Canton of Geneva, Switzerland, 2013. International World Wide Web Conferences Steering Committee.
- [HW79] J. A. Hartigan and M. A. Wong. Algorithm as 136: A k-means clustering algorithm. *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, 28(1):100–108, 1979.



# References II

- [JD88] Anil K. Jain and Richard C. Dubes. *Algorithms for Clustering Data*. Prentice Hall, 1988.
- [Kle98] Jon M. Kleinberg. Authoritative sources in a hyperlinked environment. In *Proceedings of the Ninth Annual ACM-SIAM Symposium on Discrete Algorithms, SODA '98*, pages 668–677, Philadelphia, PA, USA, 1998. Society for Industrial and Applied Mathematics.
- [Kle99] Jon M. Kleinberg. Authoritative sources in a hyperlinked environment. *J. ACM*, 46(5):604–632, September 1999.
- [Llo06] S. Lloyd. Least squares quantization in pcm. *IEEE Trans. Inf. Theor.*, 28(2):129–137, September 2006.
- [Mac67] J. MacQueen. Some methods for classification and analysis of multivariate observations. In *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Statistics*, pages 281–297, Berkeley, Calif., 1967. University of California Press.
- [MBKK15] Radek Mařík, Pavel Bezpalec, Jan Kučerák, and Lukáš Kencl. Revealing viber communication patterns to assess protocol vulnerability. In *2015 International Conference on Computing and Network Communications (CoCoNet) Leonia, NJ 07605: EDAS Conference Services*, volume ISBN 978-1-4673-7308-1, pages 502–510, 2015.
- [MD15] Radek Mařík and Veronika Dulíková. *Mathematical Formalization of Society Complexity*, chapter Povaha změny: Bezpečnost, rizika a stav dnešní civilizace, pages 98–129. Praha Vyšehrad, ISBN 978-80-7429-641-3, 2015. (in Czech).
- [New06] M. E. J. Newman. Modularity and community structure in networks. *Proceedings of the National Academy of Sciences*, 103(23):8577–8582, 2006.
- [New10] M. Newman. *Networks: an introduction*. Oxford University Press, Inc., 2010.
- [PVG<sup>+</sup>11] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.



# References III

- [STE07] Jerry Scripps, Pang-Ning Tan, and Abdol-Hossein Esfahanian. Node roles and community structure in networks. In *Proceedings of the 9th WebKDD and 1st SNA-KDD 2007 Workshop on Web Mining and Social Network Analysis*, WebKDD/SNA-KDD '07, pages 26–35, New York, NY, USA, 2007. ACM.
- [Weh13] Stefan Wehrli. Social network analysis, lecture notes, December 2013.
- [XW05] Rui Xu and D. Wunsch. Survey of clustering algorithms. *IEEE Transactions on Neural Networks*, 16(3):645–678, May 2005.

