Machine Learning for Graphs and Sequential Data

Graphs – Graphs & Networks

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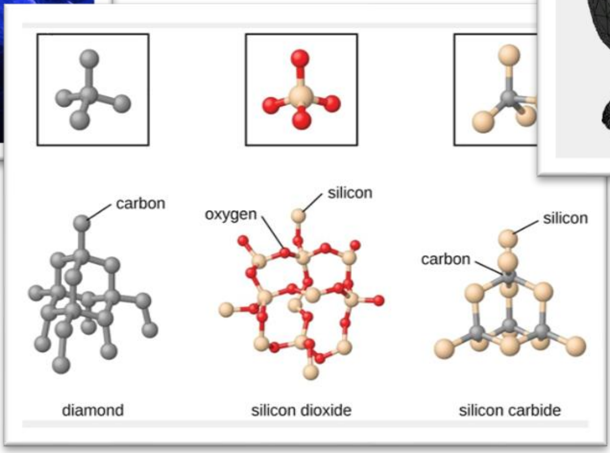
Summer Term 2023

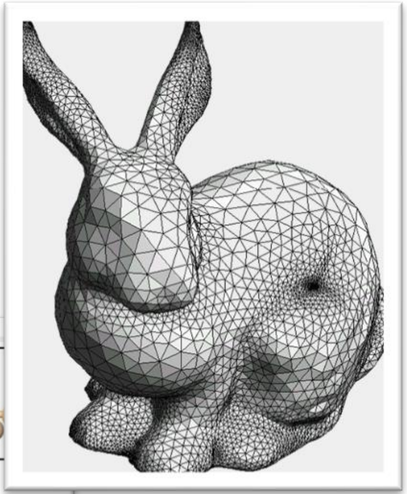
Data Analytics and
Machine Learning

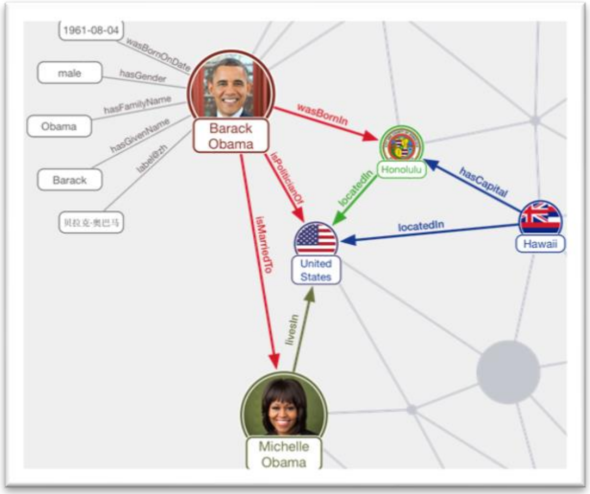
Roadmap

- **Chapter: Graphs**
  1. **Graphs & Networks**
     - **Motivation & Definitions**
     - Properties of Real Networks
  2. Generative Models
  3. Ranking
  4. Clustering
  5. Classification (Semi-Supervised Learning)
  6. Node/Graph Embeddings
  7. Graph Neural Networks (GNNs)

Why Should We Care?







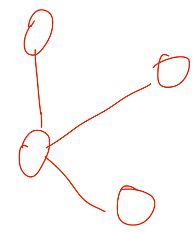
- Web: hyper-text graph
- Information retrieval:
  bi-partite graphs (documents-terms)
- E-commerce: User-Product graphs

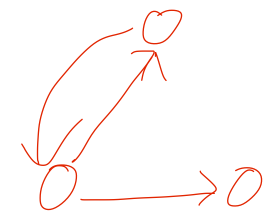
Data Analytics and Machine Learning

Why Should We Care?

- ‘Viral’ marketing, News propagation
- Computer network security: email/IP traffic and anomaly detection
- Ranking of search results
- Fraud detection in e-commerce systems
- Drug discovery, molecule property prediction
- Scene graph analysis
- …

Basic Definition





- Plain/simple graph $G = (V, E)$
  - Set of nodes V
  - Set of edges $E \subseteq V \times V$ // for undirected graphs: $(i,j) \in E \Leftrightarrow (j,i) \in E$
- Equivalent representation via (binary) adjacency matrix $A \in \{0,1\}^{|V| \times |V|}$

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad 4 \times 4 \quad \{0,1\}$$

- Multiple extensions possible
  - weighted graphs (node weights, edge weights)
  - attributed graphs (multi-dimensional vectors assigned to nodes/edges)
  - temporal graphs (timestamp associated with node/edge)

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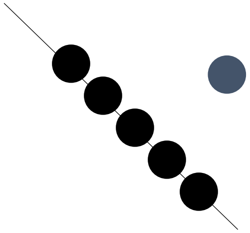
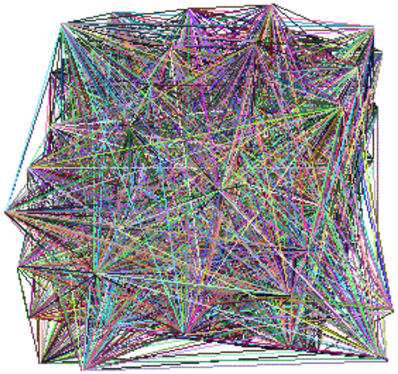
How are real networks structured?

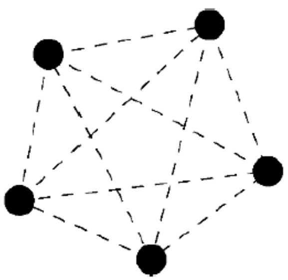
- What does the Internet look like?
- What does Facebook look like?
- What is 'normal'/'abnormal'? ⇒ e.g. unusual behaviour
- Which patterns/laws hold?
  - To spot anomalies (rarities), we have to discover patterns
  - **Large datasets** reveal patterns/anomalies that may be invisible otherwise…





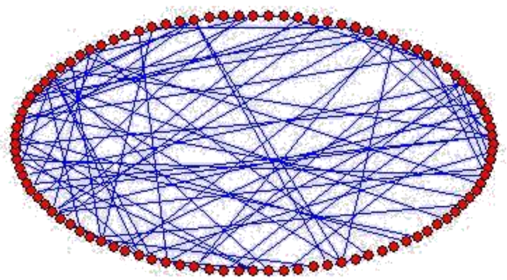
Are real graphs random?

- Erdös-Renyi Random Graph Model
  - Start with N (isolated) nodes
  - For every pair $v1, v2 \in V$ add an edge with probability p
  - Every edge occurs with equal probability

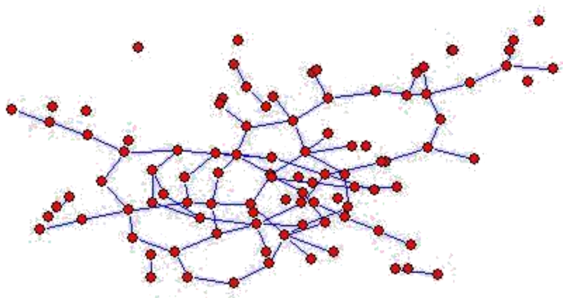


- Example: 100 nodes, avg degree = 2

before layout



after layout



- No obvious patterns

Laws and Patterns

- Q: Are real graphs random?
- A: NO!
  - Diameter
  - in- and out- degree distributions
  - other (surprising) patterns

- So, let's look at the data

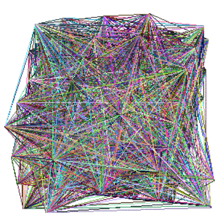
Power Law Distributions

- Gaussian distributions are common in nature
- In networks, however, a **power law distribution** often explains the data better
- Example: Power law in the degree distribution

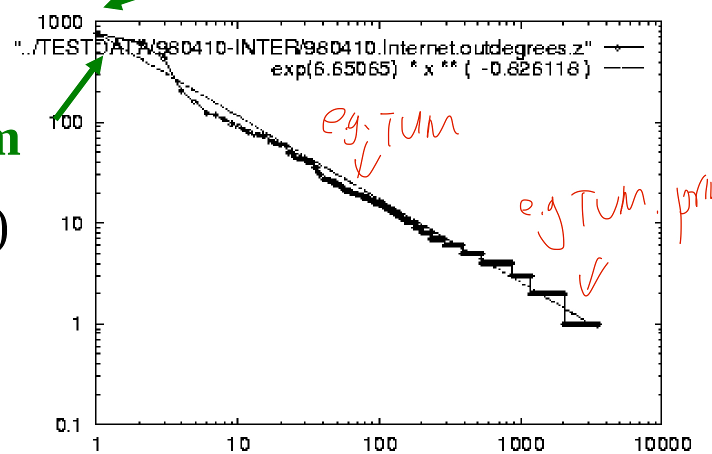
internet domains

att.com

ibm.com



log(degree)



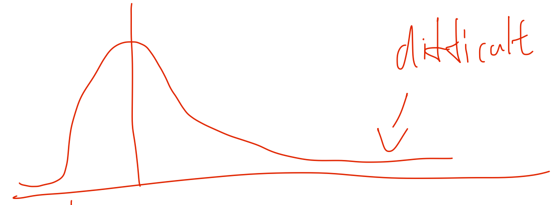
e.g. TUM

e.g. TUM. prime . . .

log(rank)

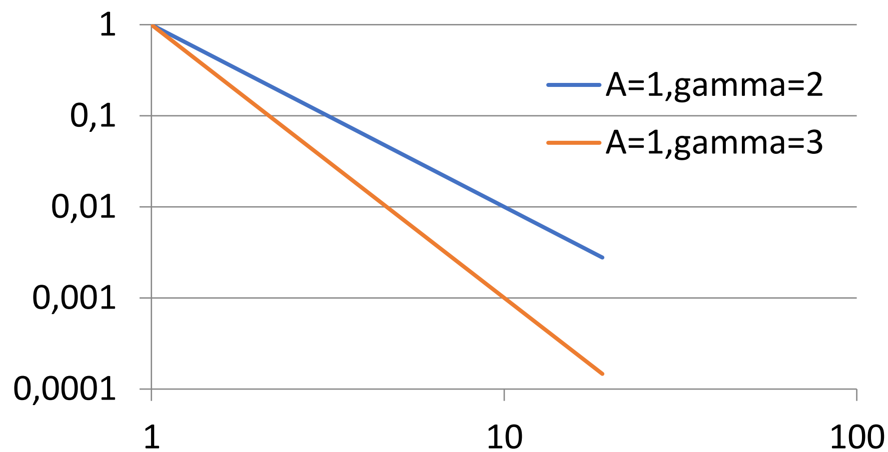
Power Law Distributions

difficult observe



- Definition Power Law:
  - Two variables x and y are related by a power law when $y(x) = Ax^{-\gamma}$ where A and γ (power law exponent) are positive constants
  - A random variable is distributed according to a power law when the probability density function (pdf) is given by $p(x) = Ax^{-\gamma}$ with $\gamma > 1$

- Note: Power law distribution looks like a line on a log-log scale
- **Characteristic: Decay of pdf is only polynomial (Gaussian: exponential)**
- → More likely to observe values far to the right of the mean
  - E.g. more likely to have nodes with a very high degree

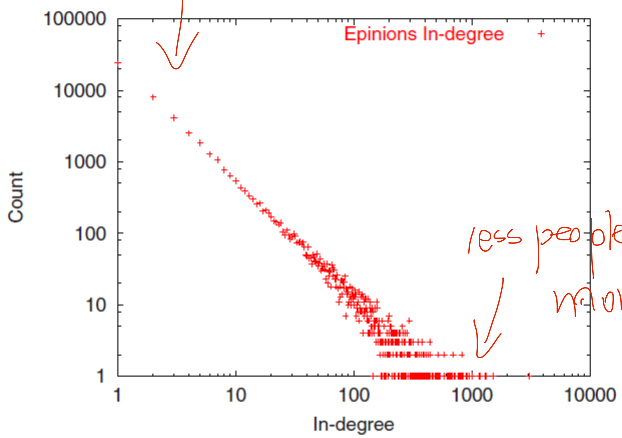


a.k.a. heavy-tailed distributions

Examples: Power Law Distributions

- "Internet AS" graph with exponent 2.1 – 2.2
- "Internet router" graph with exponent 2.48
- Citation graphs with exponent 3
- Epinions (who-trust-whom)
- …

more people with less followers



less people with more follower

(a) Epinions In-degree

- Note: Graphs with degree distributions following a power law are called **scale-free**
  - $y(a \cdot x) = b \cdot y(x)$ // y(x)=number of nodes with degree x

Important Remark

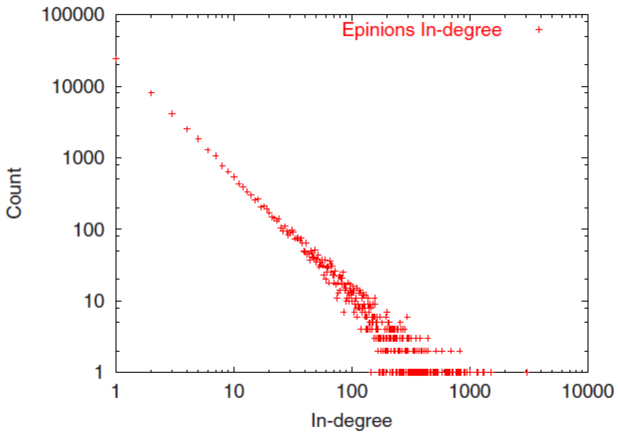
重要提示：我们并不声称数据的基本分布是幂律分布

而是：在许多情况下，幂律分布是对我们观察到的情况的良好描述/拟合（或近似）。

- Important: We do not claim that the data's underlying distribution is a power law distribution
- Instead: In many cases a power law distribution is a **good description/fit** (or approximation) of what we observe
  - usually deviations to power law distribution are observed (to different degrees)
  - other models: exponential cutoff, lognormal distributions

- 通常观察到对幂律分布的偏离（不同程度）。

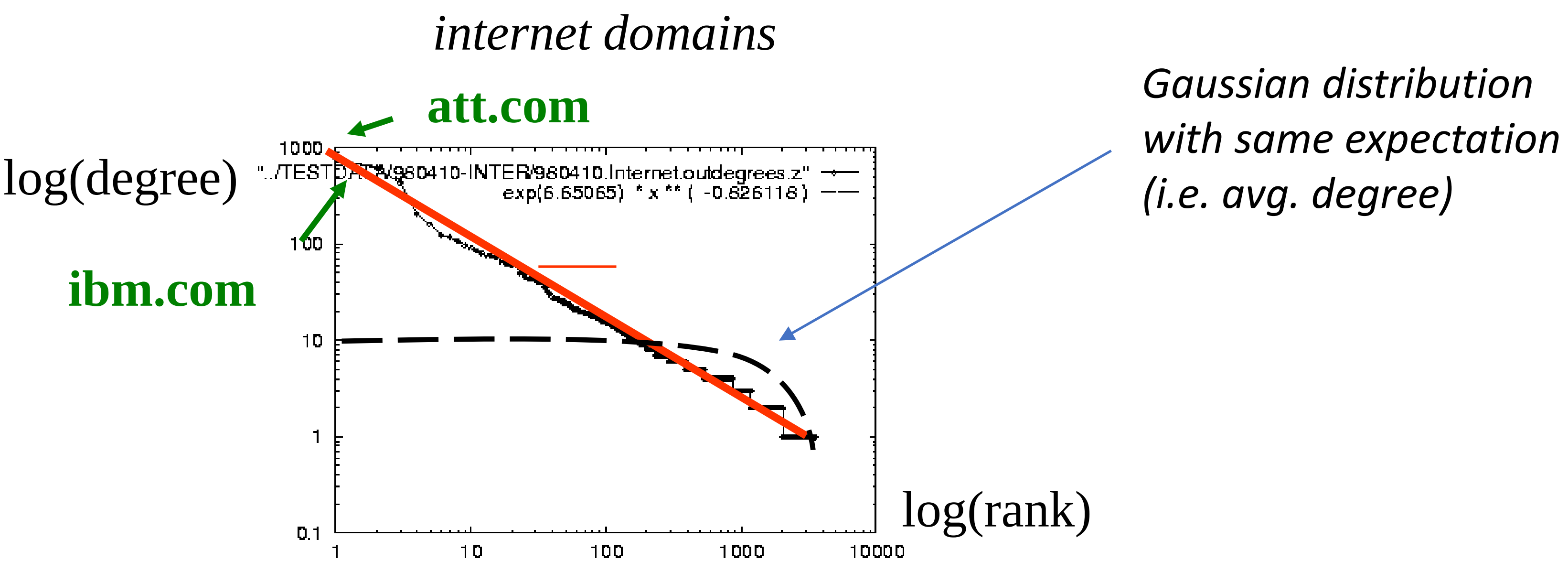
- 其他模型：指数截止，对数正态分布



(a) Epinions In-degree

"Gaussian Trap"

- Q: So what?
- A1: Be careful when writing algorithms!
  - Example: # of two-step-away pairs (= friends of friends)
    - O(d_max ^2)   ~ 10M^2
      for storage: ~0.8PB → a data center(!)

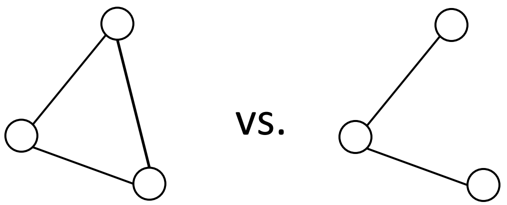


Patterns and Algorithms

- Q: So what?
- A2: Patterns allow to design new algorithms!

Example: Clustering Coefficient

- Real social networks have a lot of triangles
  - Friends of friends are friends



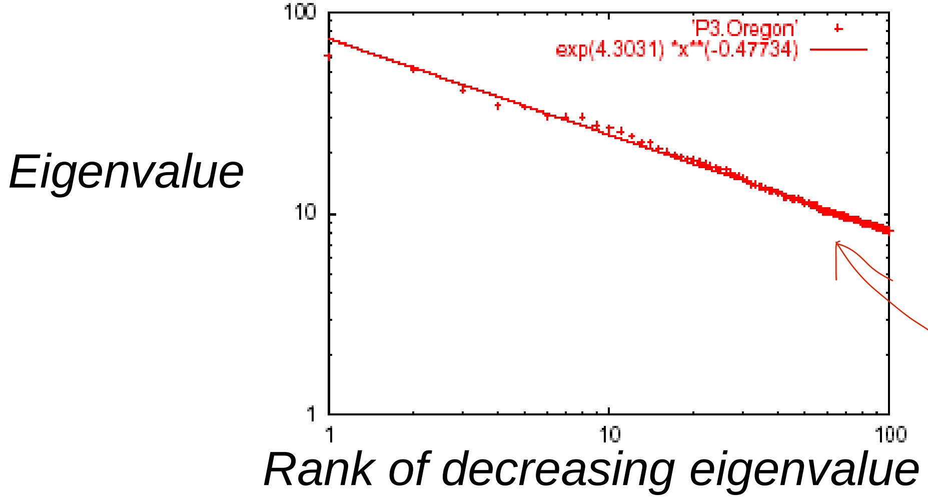
- Clustering Coefficient
  - $\boxed{C = \frac{3 \cdot number\ of\ triangles}{number\ of\ connected\ triplets}}$

More triangles bigger C

  - Real-world networks often show large clustering coefficients
    → Strong community structure
- Computation of clustering coefficient requires computation of triangles
  - But: **triangles are expensive to compute** (3-way join)

Efficient Triangle Counting

- How to efficiently estimate the number of triangles?
  - Let's look at some patterns…
- Recap: Adjacency matrix $\boldsymbol{A} \in \{0,1\}^{N \times N}$
  - $a_{ij} = 1$ if there is an edge between i and j, 0 otherwise
- Recap: Eigenvalue decomposition $\boldsymbol{A}\,\boldsymbol{x} = \lambda\,\boldsymbol{x}$
- Observer: Power law in the eigenvalues of the adjacency matrix



Exponent = slope

$E = -0.48$

also power law

many eigenvalue = small a

Efficient Triangle Counting

- How does this help?

1. Some nice fact (easy to show):
   - number of triangles $= \frac{1}{6} trace(A^3) = \frac{1}{6} \sum_i \lambda_i^3$
     adjacent matrix
   - λ_i = eigenvalues of adjacency matrix A

2. Eigenvalues follow power law (highly skewed)
   - we only need the top few (largest) eigenvalues!
   - how can we compute them efficiently?

Recap: Power Iteration

- Eigenvalues are important for many ML/data mining tasks
  - PCA, Ranking of Websites, Community Detection, …
  - How to compute them efficiently?

- Power iteration (a.k.a. Von Mises iteration)
  - Iterative approach to compute **a single** eigenvector
- Let X be a matrix and v be an arbitrary (normalized) vector
  - Iteratively compute $v \leftarrow \frac{X \cdot v}{\|X \cdot v\|}$ until convergence
    - in each step, v is simply multiplied with X and normalized
  - **v converges to the eigenvector of X with greatest absolute value**
  - Highly efficient for sparse data

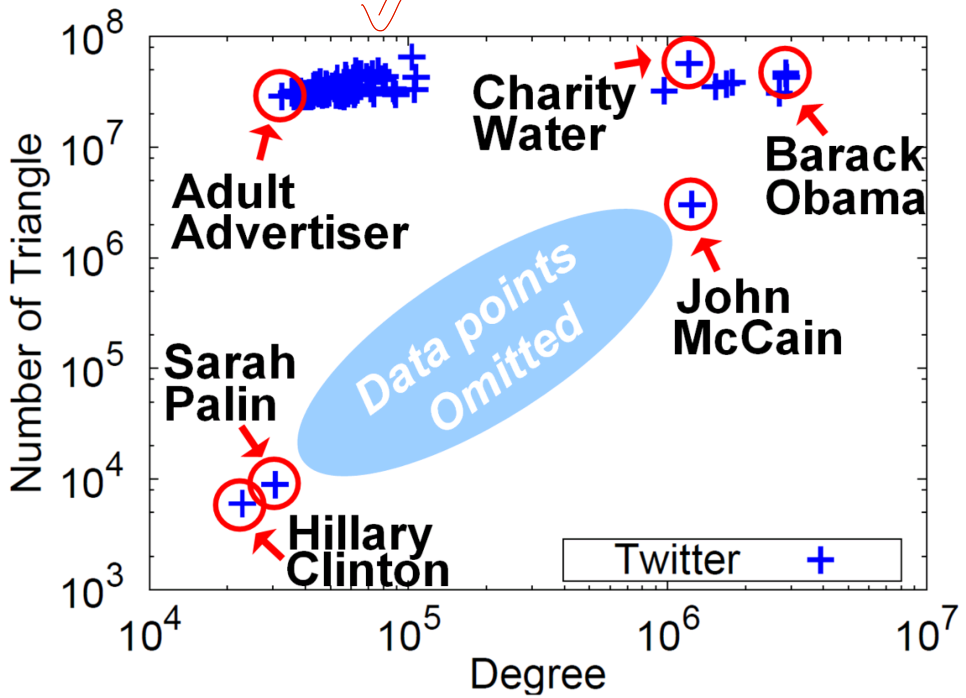
Recap: Power Iteration

- Convergence:
  - Linear convergence with rate $|\lambda_2/\lambda_1|$
  - Fast convergence if first and second eigenvalue are dissimilar

- How to find **multiple (the k largest) eigenvectors**?
  - Let us focus on symmetric matrices X
  - Eigenvalue decomposition leads to: $X = \Gamma \cdot \Lambda \cdot \Gamma^T = \sum_{i=1}^{d} \lambda_i \cdot \gamma_i \cdot \gamma_i^T$
  - Define deflated matrix: $\hat{X} = X - \lambda_1 \cdot \gamma_1 \cdot \gamma_1^T$
    - $\hat{X}$ has the same eigenvectors as X except the first one has become zero
  - ➢ Apply power iteration on $\hat{X}$ to find the second largest eigenvector of X

Example: Analysis of Twitter

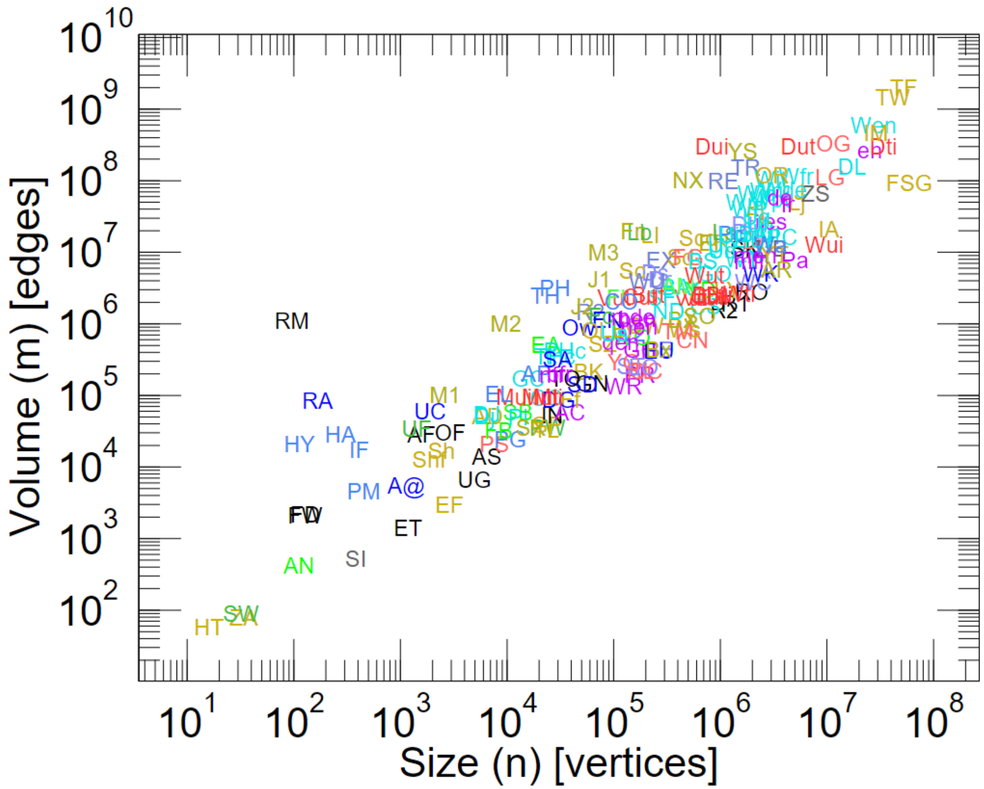
unusual = low followers with high count



- Anomalous nodes in Twitter (~ 3 billion edges)
- [U Kang et. al., PAKDD'11]

Real Graphs are Sparse

- N^2 possible edges for a graph with N nodes
- However, real-world graphs are very sparse $\mathrm{E} \ll N^2$
- Instead of $\mathrm{E} = O(N^2)$, we see $\mathrm{E} = O(N^{\alpha})$ with α significantly less than 2



Every "XX" is a real world network

Note the log-log scale

$\alpha \approx 1.4$

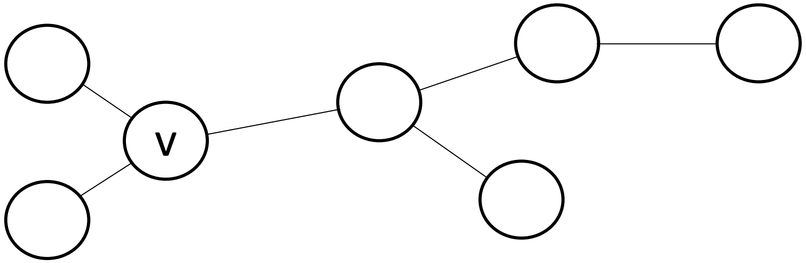
Small World Phenomenon

- Famous experiment by Travers and Milgram [TM1969]
  - Setup: Try to reach a random person by sending a chain letter
  - Result: The average length of chains that reach the person was six
  - → Length very small compared to number of participants
  - → „Small world phenomenon"; „six degrees of separation"

- Ways to measure this phenomenon
  - Characteristic path length
  - Average diameter
  - Effective diameter/Eccentricity

Characteristic Path Length & Average Diameter

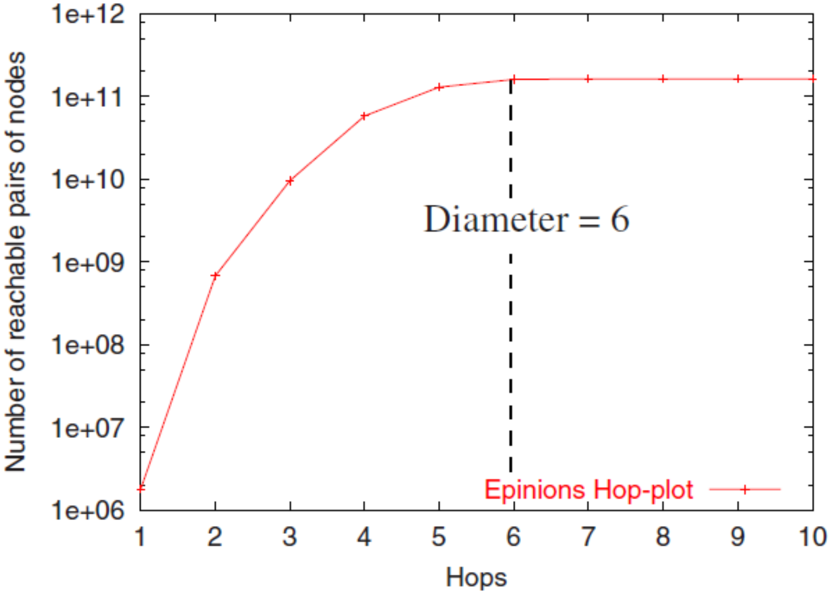
- Characteristic path length
  - For each starting node $v \in V$ consider the shortest path to every other node
  - Take the average length of all these paths
  - Consider average path length for all starting nodes and take the median
  - $\underset{v \in V}{\text{median}} \left\{ \frac{1}{|V|} \sum_{v_j \in V} len(p_{min}(v, v_j)) \right\}$



- Average diameter
  - Similar to above but use (in last step) the mean instead of the median
  - $\frac{1}{|V|} \sum_{v \in V} \frac{1}{|V|} \sum_{v_j \in V} len(p_{min}(v, v_j))$

Effective Diameter / Eccentricity & Hop-plot

- Let $N_h(u)$ be the number of nodes reachable from u via h hops
  - $N_h(u) = \{v \in V \mid len(p_{min}(u,v)) \leq h\}$
- The total neighborhood size N_h is the sum over all starting nodes
  - $N_h = \sum_{u \in V} |N_h(u)|$
- Hop-plot: Plot of N_h versus h



- Effective diameter (or Eccentricity)
  - Minimum number of hops in which some fraction (e.g. 90%) of all connected pairs of nodes can reach each other
  - $\min\{k \in \mathbb{N} \mid N_k \geq 0.9 \cdot |V|^2\}$ 所有连接的节点对中有一部分（如90%）可以到达对方的最小跳数。
  - **Advantage: Also works for disconnected graphs**

Importance of „Network Laws“

- Laws describing „normal“ networks are important for:
- Design of algorithms
- Detection of abnormal/interesting patterns
  - Abnormalities deviate from the „normal“ patterns
  - Prerequisite: specify what is normal
- Development of graph generators
  - Often: real world data not public available; or just small excerpts
  - Use synthetic data to test algorithms
  - Requirement: generate synthetic but realistic graphs
- Simulation studies
  - E.g. test next-generation internet protocol on graph „similar“ to what Internet will look like a few years into the future

Questions

- How much memory do you need to store the edges of a graph with 1000 nodes and 10,000 edges in a dense adjacency matrix? How much for a sparse matrix?

- What is the average degree in an Erdös-Renyi graph with edge probability p? And in a real world sparse graph with $O(\mathrm{E}) = O(N^{\alpha})$?

Reading Material

- "Graph Mining: Laws, Tools, and Case Studies" by Deepayan Chakrabarti, Christos Faloutsos

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