Graphs in Machine Learning

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DeepMind Paris, France

Collaborators: Achraf Azize,
Michal Valko

Partially based on material by: Andreas Krause,
Branislav Kveton, Michael Kearns

Administrivia

7/8 lectures 2x(50m + 10m break)

3 recitations (TDs) 2h + 2 weeks to deliver homework

TA: Achraf Azize

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Time: Mondays 16:00-18:00, 23/1 to 3/4

Place: online, link posted on Piazza

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Validation: grades from TDs

Piazza for Q&A's

Contact, online class discussions, and announcements:

- registration for the class
- register with your **school** email and **full name**
- online course discussions and announcements
- questions and answers about the material and logistics
- **students encouraged to answer each others' questions**
- homework assignments
- draft of the slides before the class

`https://piazza.com/ens_cachan/spring2023/mvagraphsml` **NO EMAILS!**

class code: **mvagraphsml** write it down right now + register with your school email

Course website:

`https://sites.google.com/view/daniele-calandriello/teaching`

Two (main) sources of graphs in ML

Natural graphs as models for networks

Constructed graphs as nonparametric basis

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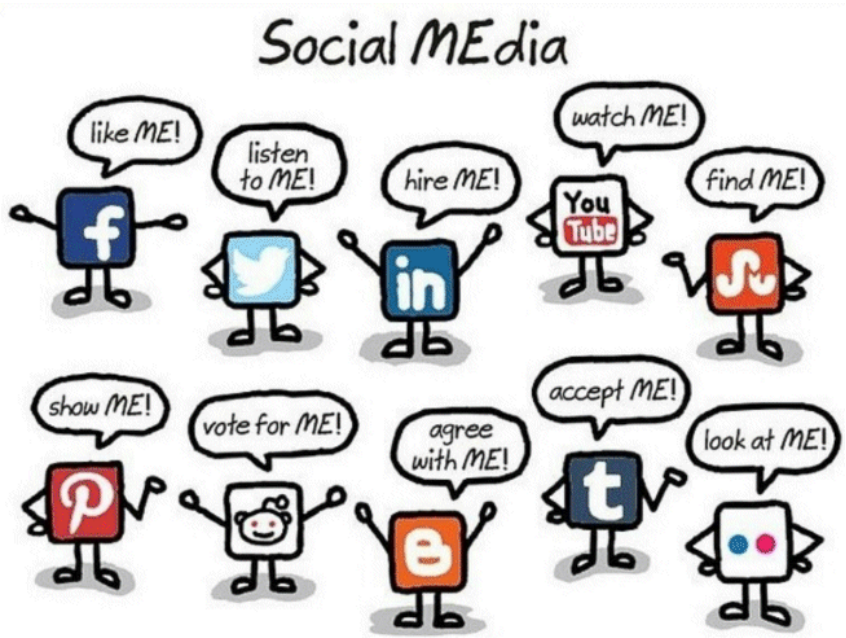
Constructed graphs as nonparametric basis

- we create (learn) the similarity structure from flat data
- it's a tool (e.g., nonparametric regularizer) to encode structural properties (e.g., independence, . . .)

Natural graphs from social networks

- people and their interactions



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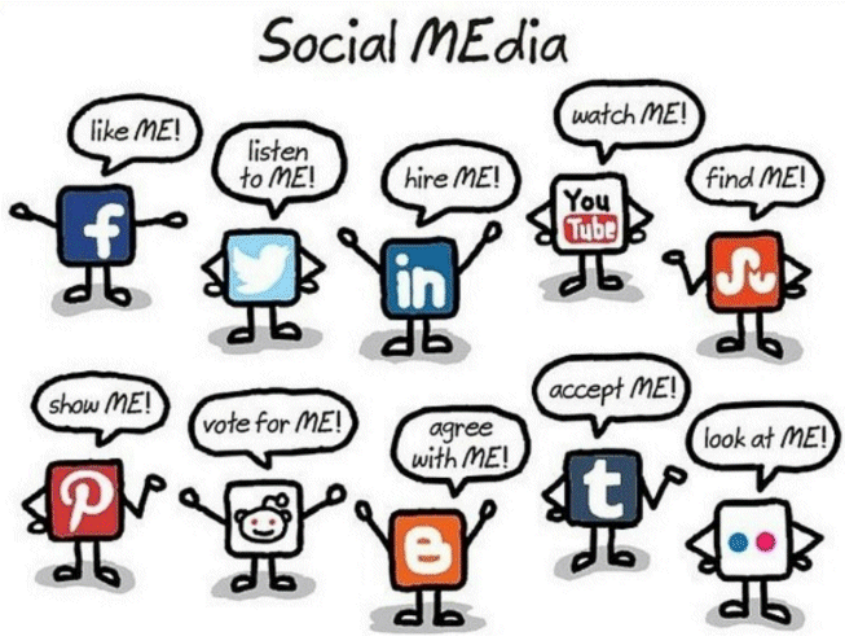

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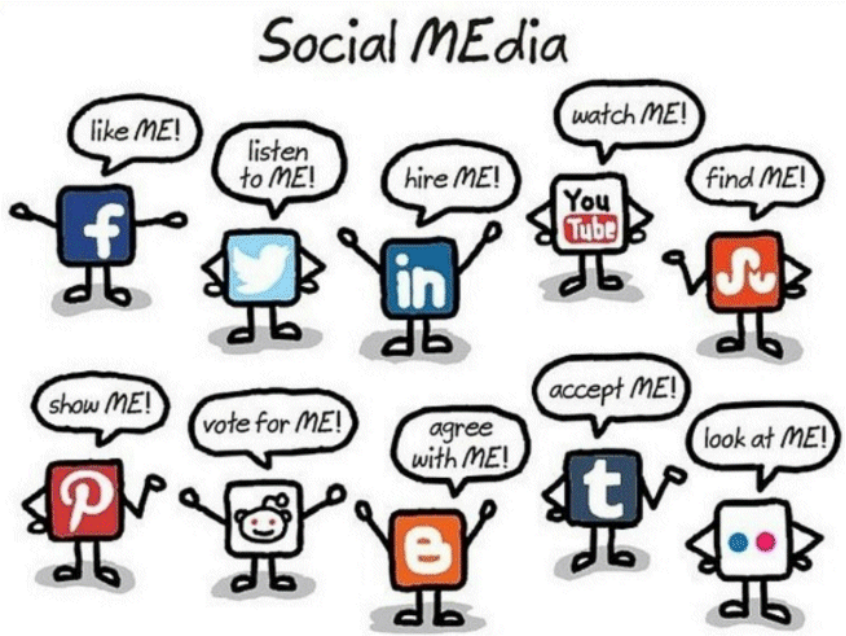

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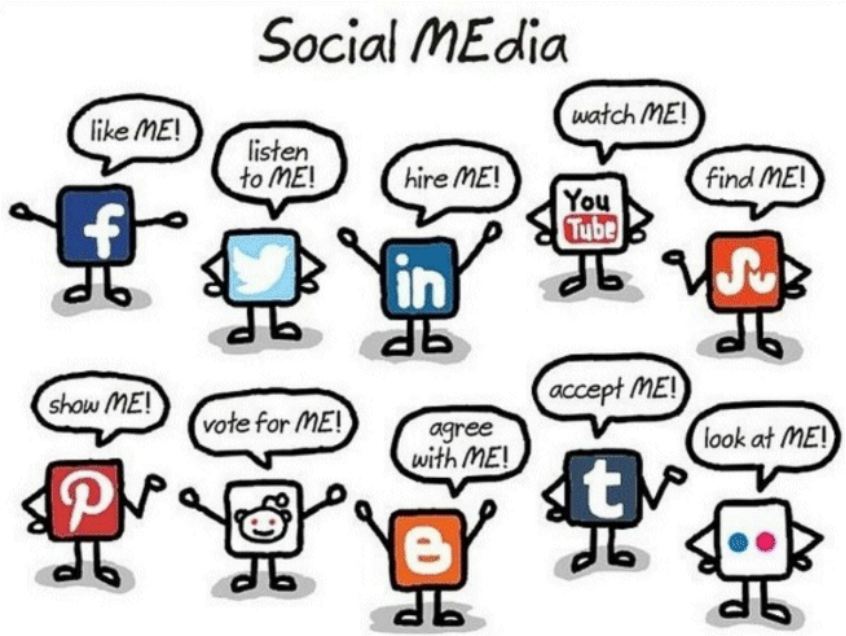

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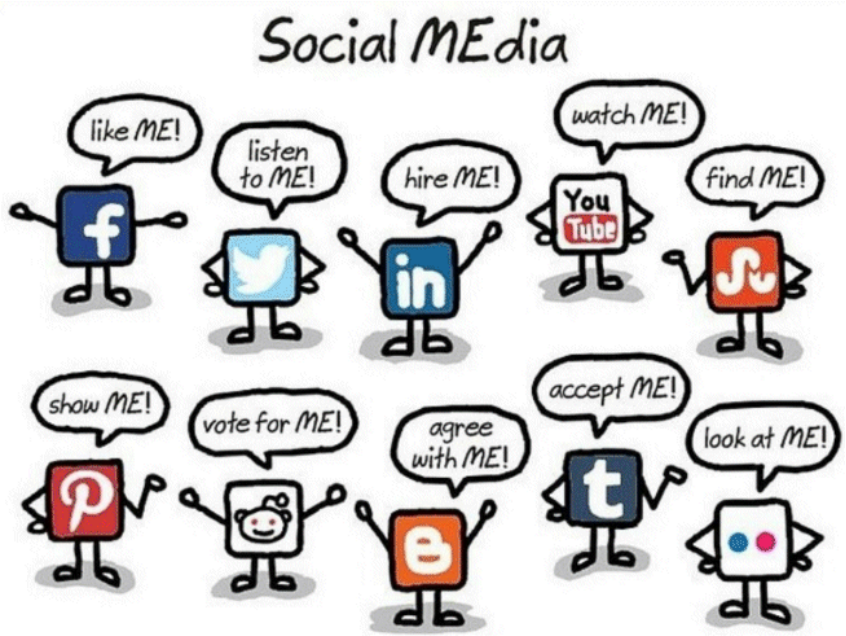
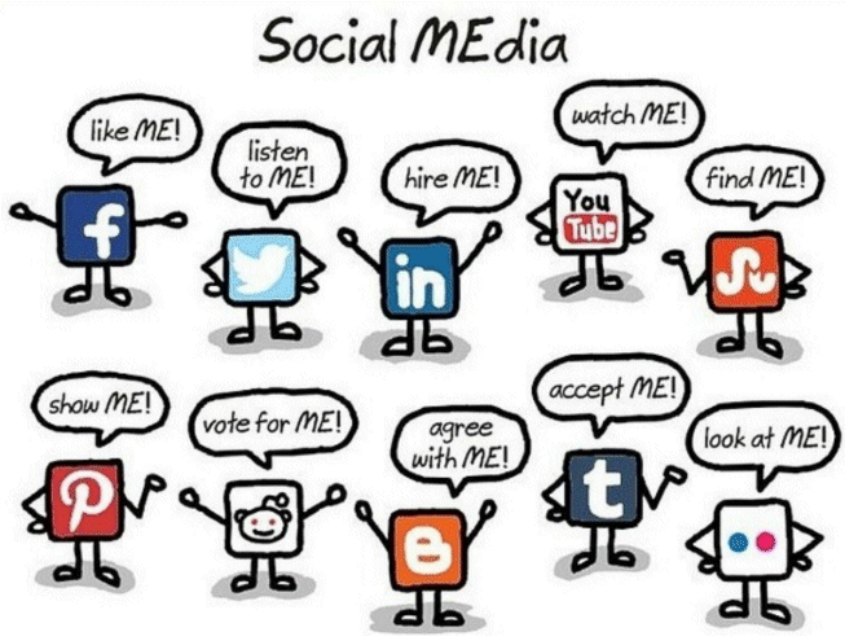
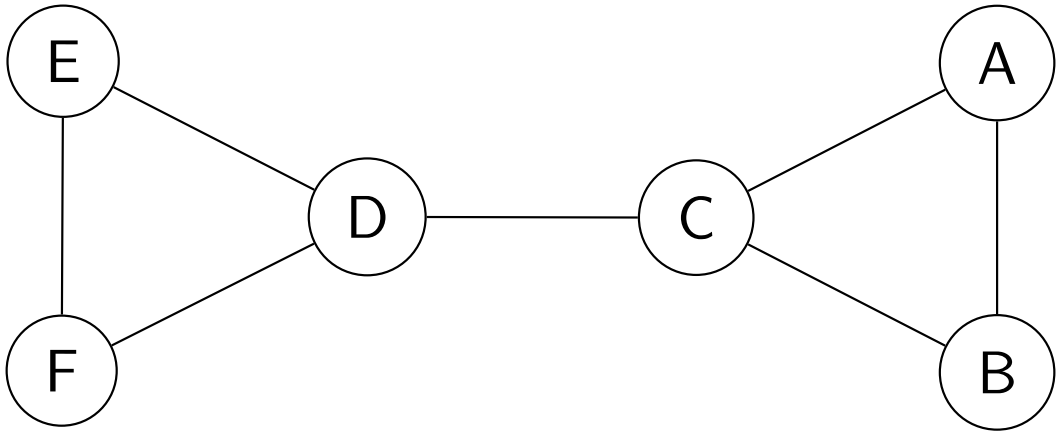


Natural graphs from social networks

- people and their interactions
- structure is rather a *phenomena*
- typical ML tasks
  - advertising
  - link prediction (PYMK)
  - find influential sources



Success story #1 Product placement - problem



Maximizing the Spread of Influence through a Social Network
`http://www.cs.cornell.edu/home/kleinber/kdd03-inf.pdf`

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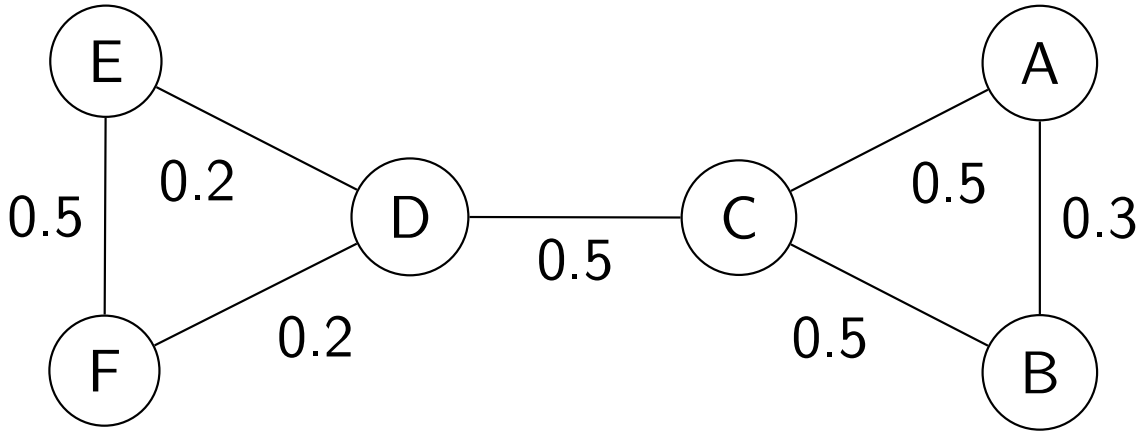

Who should get free cell phones?

$V = \{$**A**lice,**B**ob,**C**harlie,**D**orothy,**E**ric,**F**iona$\}$

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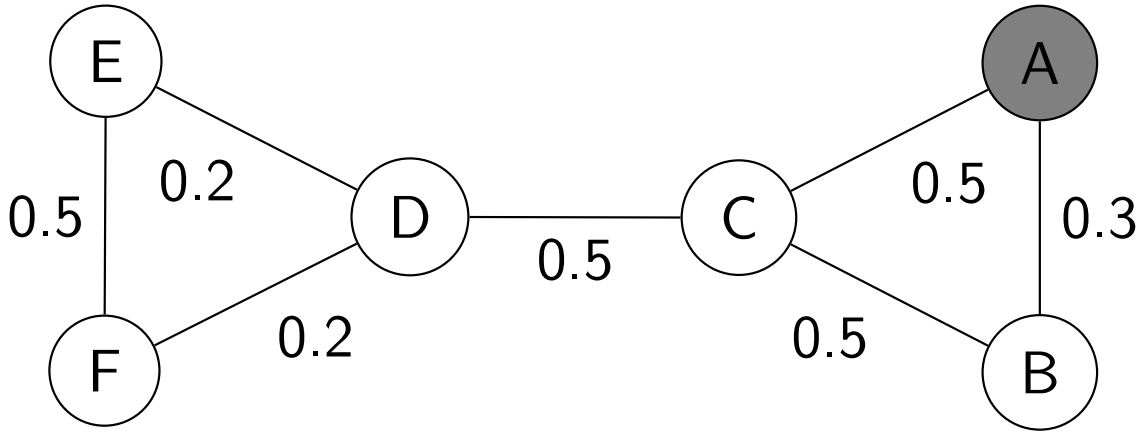

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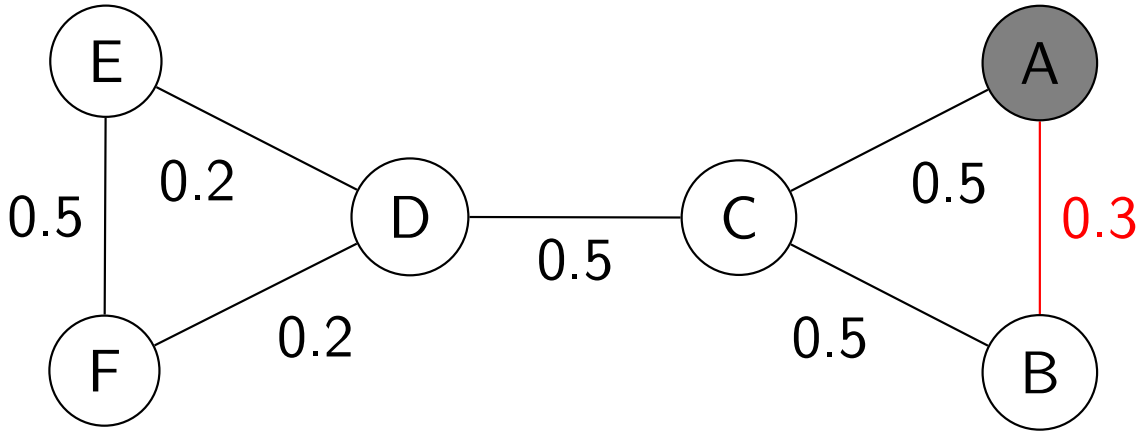

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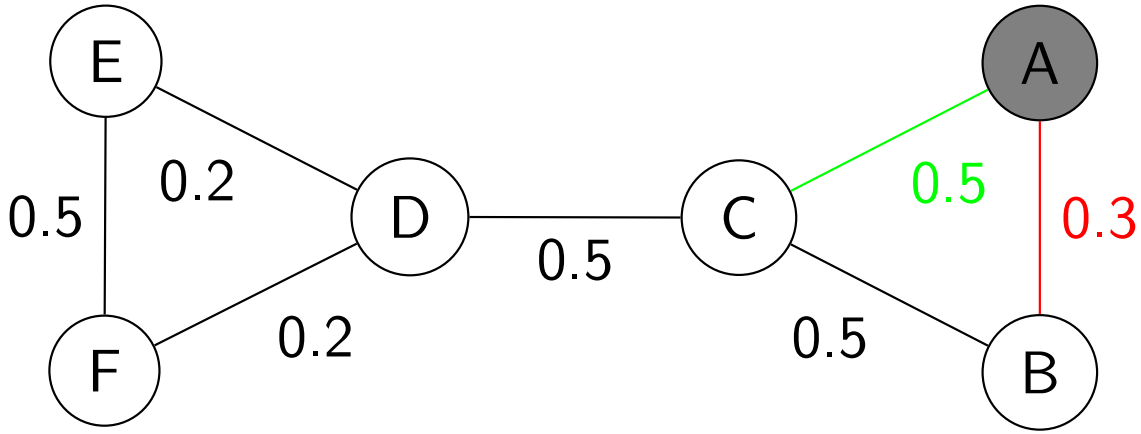

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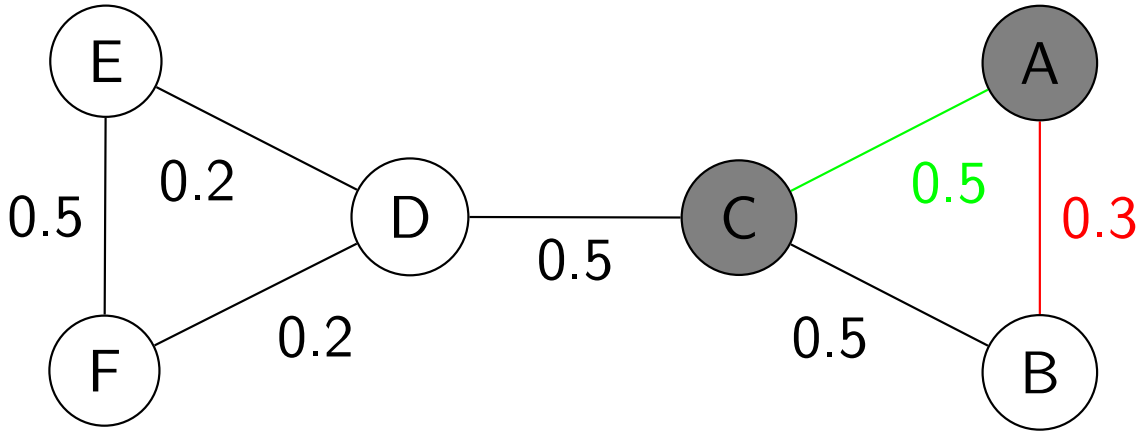

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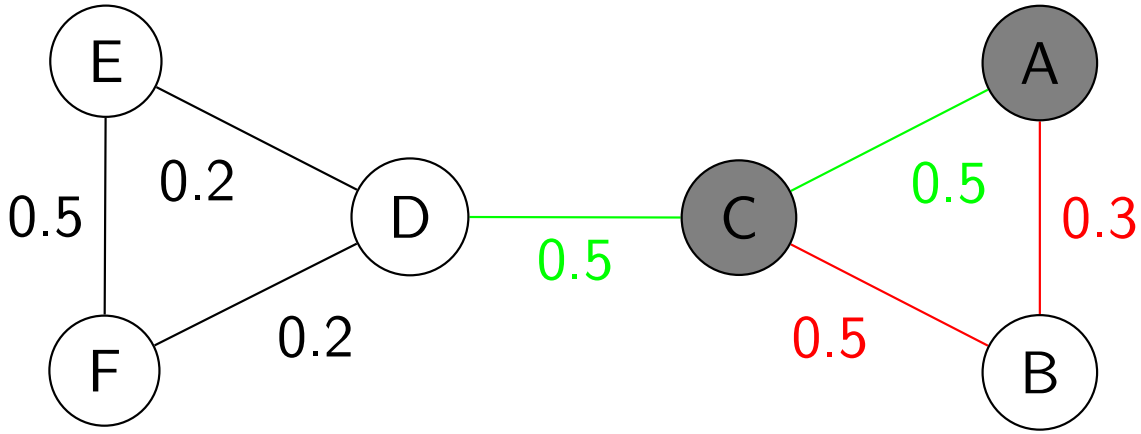

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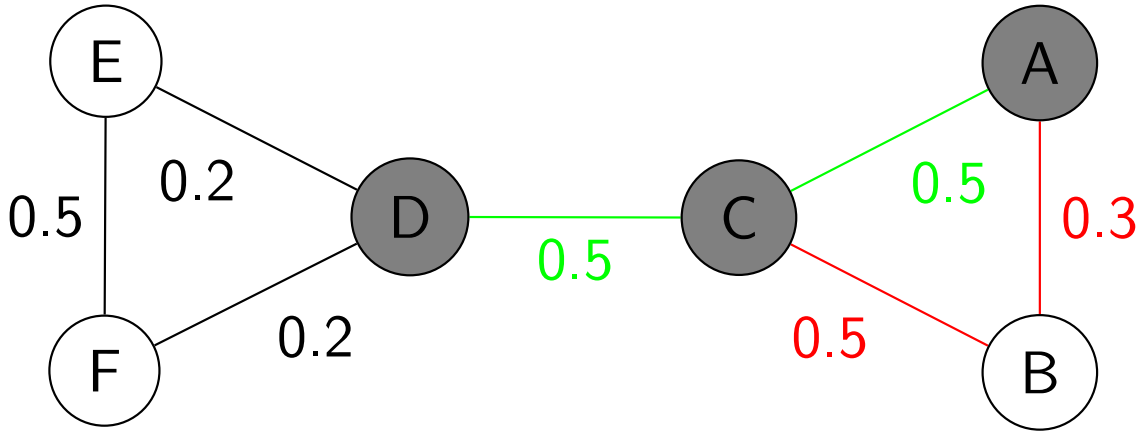

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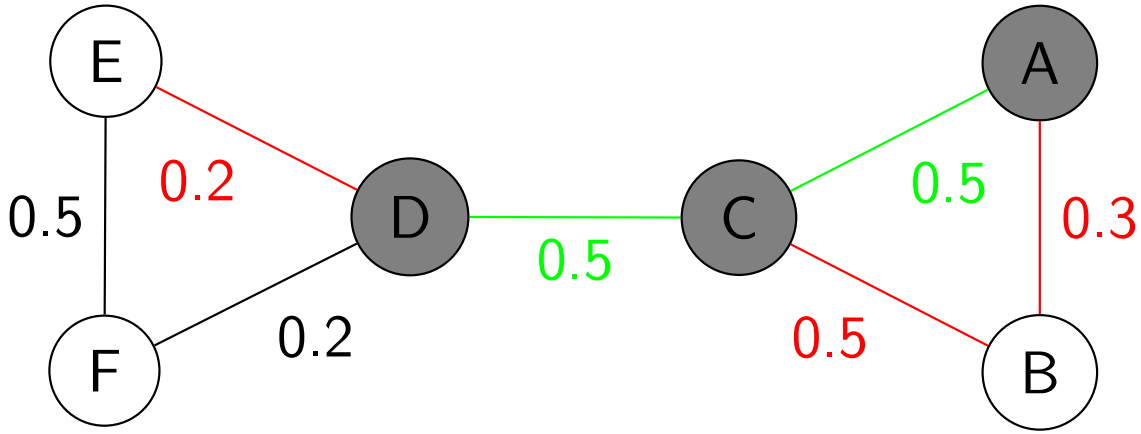

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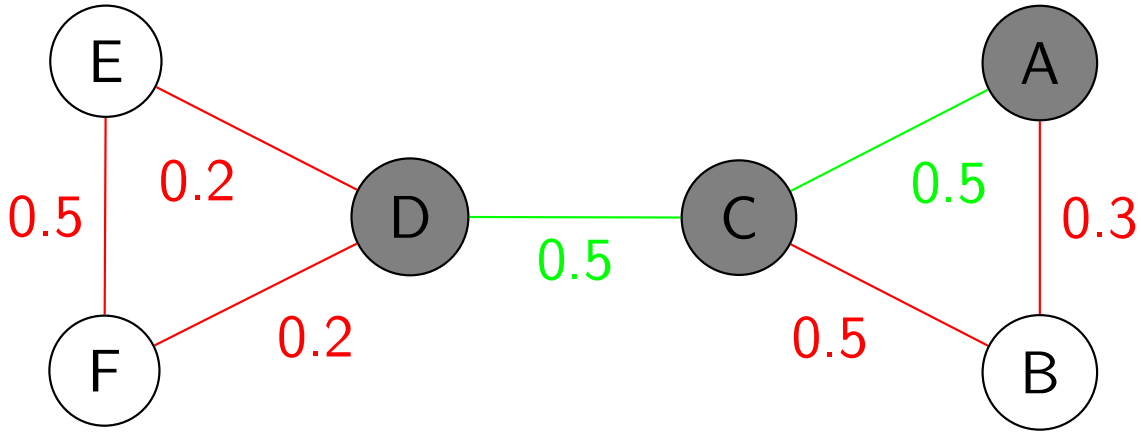

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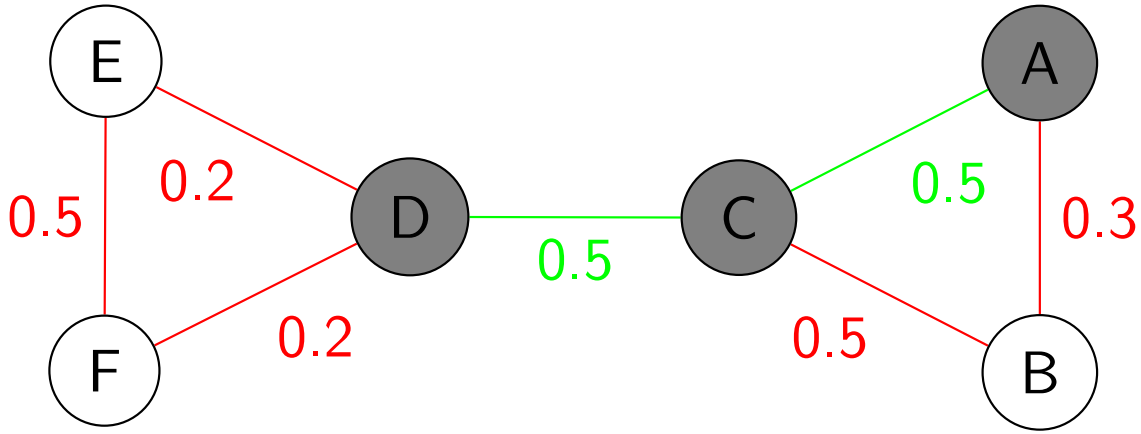

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How would you choose the target customers?

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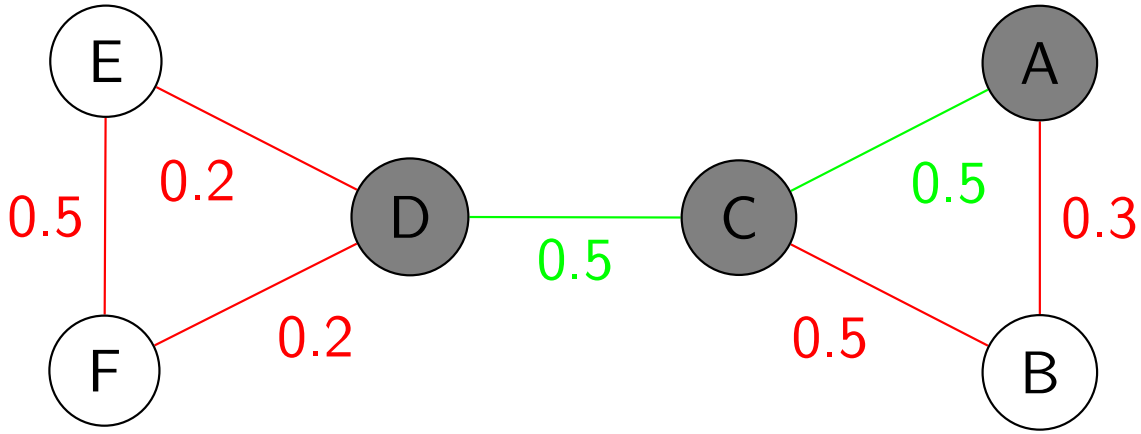

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highest degree, close to the center, . . .

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Submodularity: modeling diminishing returns

Example: $S = \{\text{stuff}\} = \{\text{bread, apple, tomato, ...}\}$

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A **set function** on a discrete set A is **submodular** if for any $S \subseteq T \subseteq A$ and for any $e \in A \setminus T$

$$f(S \cup \{e\}) - f(S) \geq f(T \cup \{e\}) - f(T)$$

Submodularity: Application

Link to our **product placement** problem on a **social network graph?**

Objective: Find $\arg\max_{S \subseteq A, |S| \leq k} f(S)$

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Let $S^\star = \arg\max_{S \subseteq A, |S| \leq k} f(S)$ where f is monotonic and submodular set function and let $S_{\texttt{Greedy}}$ be a **greedy solution**.

$$\text{Then} \quad f(S_{\texttt{Greedy}}) \geq \left(1 - \frac{1}{e}\right) \cdot f(S^\star).$$

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Other applications: information, graph cuts, covering, ...

Submodularity: `Greedy` algorithm

Input:
  k: the maximum allowed cardinality of the output
  V: a ground set
  f: a monotone, non-negative, and submodular function
Run:
$S_0 = \emptyset$
for $i = 1$ **to** k **do**
  $S_i \leftarrow S_{i-1} \cup \left\{ \arg\max_{a \in V \setminus S_{i-1}} \left[f\left(\{a\} \cup S_{i-1}\right) - f\left(S_{i-1}\right) \right] \right\}$
end for
Output:
  Return $S_{\texttt{Greedy}} = S_k$

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Submodularity: Approximation guarantee of `Greedy`

Let S_i be the i-th set selected by `Greedy`. We show

$$f(S^\star) - f(S_{i-1}) \leq f(S^\star \cup S_{i-1}) - f(S_{i-1})$$

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& \leq f(a \cup S_{i-1}) - f(S_{i-1}) + f(S^\star / a \cup S_{i-1}) - f(S_{i-1}) \\
& \leq \sum_{a \in S^\star \setminus S_{i-1}} \left(f(\{a\} \cup S_{i-1}) - f(S_{i-1}) \right) \\
& \leq \sum_{a \in S^\star \setminus S_{i-1}} \left(f(S_i) - f(S_{i-1}) \right) \leq k \left(f(S_i) - f(S_{i-1}) \right)
\end{aligned}
$$

Difference from the optimum of $S_{\texttt{Greedy}} = S_k$ after the k-th step ...

$$
\begin{aligned}
f(S^\star) - f(S_k) &= f(S^\star) - f(S_{k-1}) - \left(f(S_k) - f(S_{k-1}) \right) \\
&\leq f(S^\star) - f(S_{k-1}) - \frac{f(S^\star) - f(S_{k-1})}{k} \\
&\leq \left(1 - \tfrac{1}{k}\right) \cdot \left(f(S^\star) - f(S_{k-1}) \right) \leq \left(1 - \tfrac{1}{k}\right)^k \cdot f(S^\star)
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Submodularity: Graph-related examples

- Influence maximization on networks (current example)

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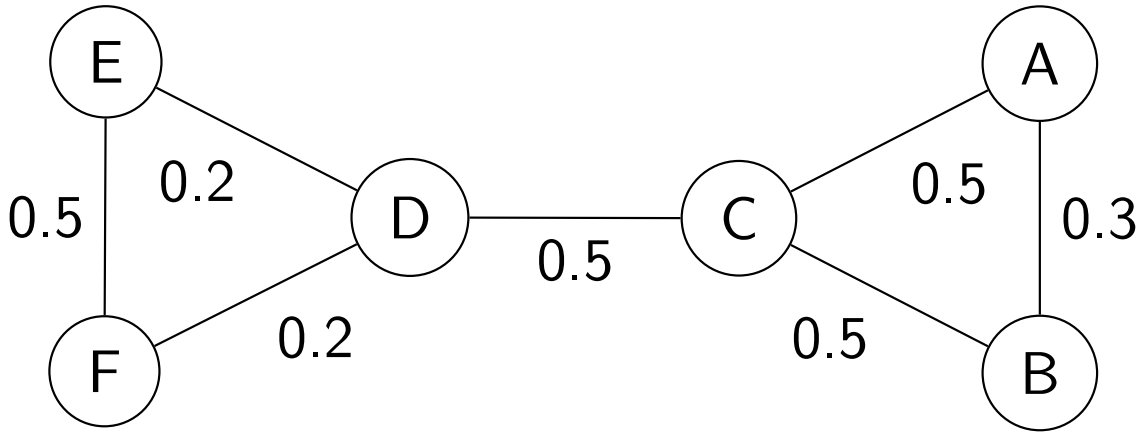
back to the influence-maximization example ...

Success story #1 Product placement - solution



Key idea: Flip coins c in advance $\rightarrow$ "live" edges

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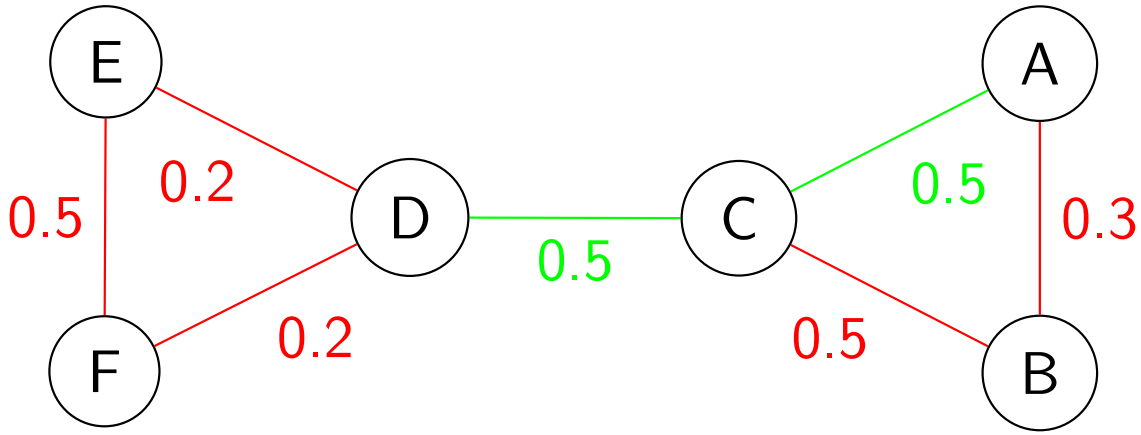

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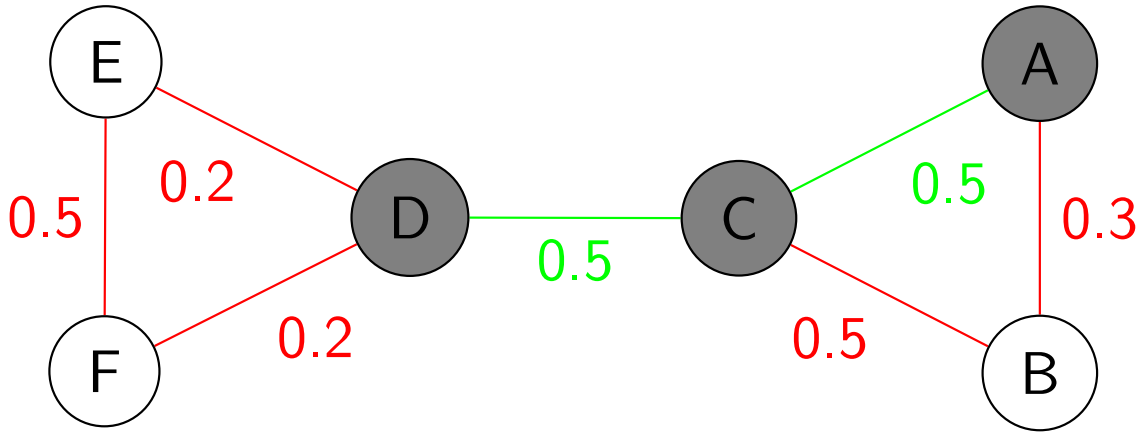

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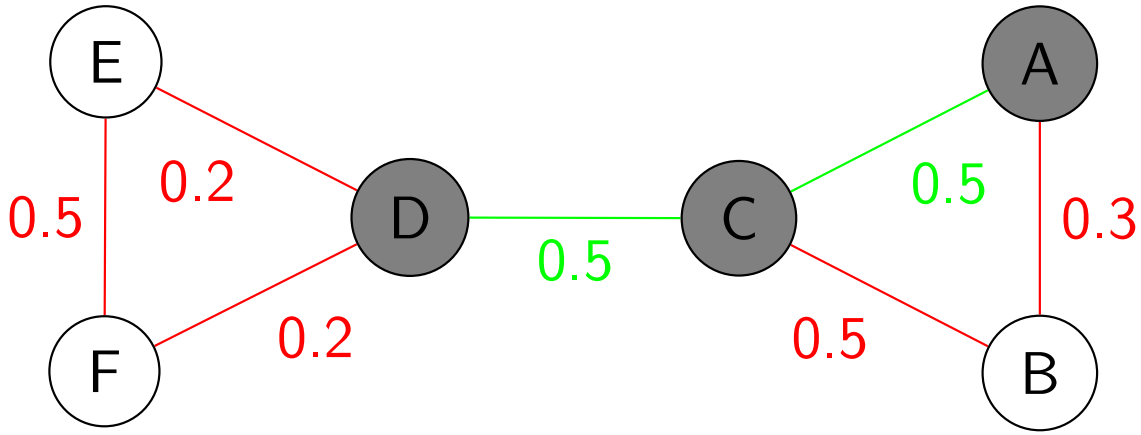

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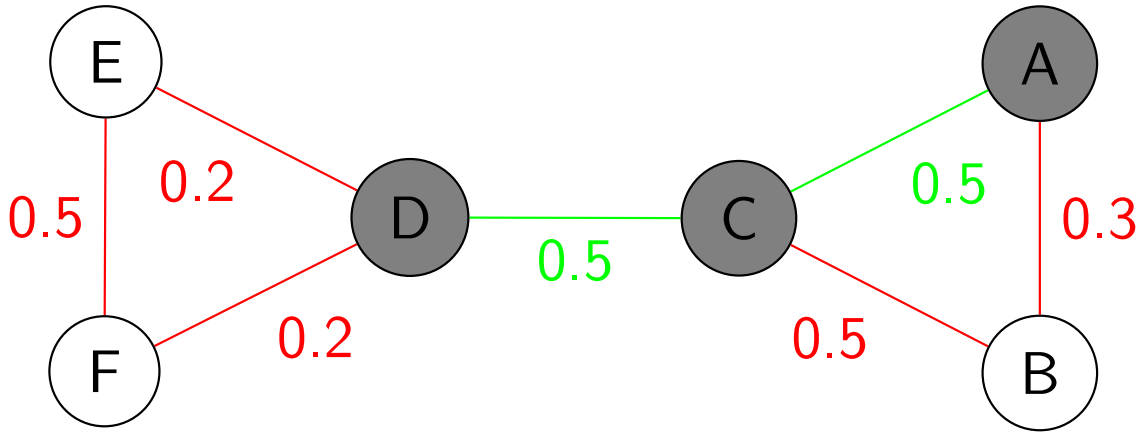

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Computational issues?

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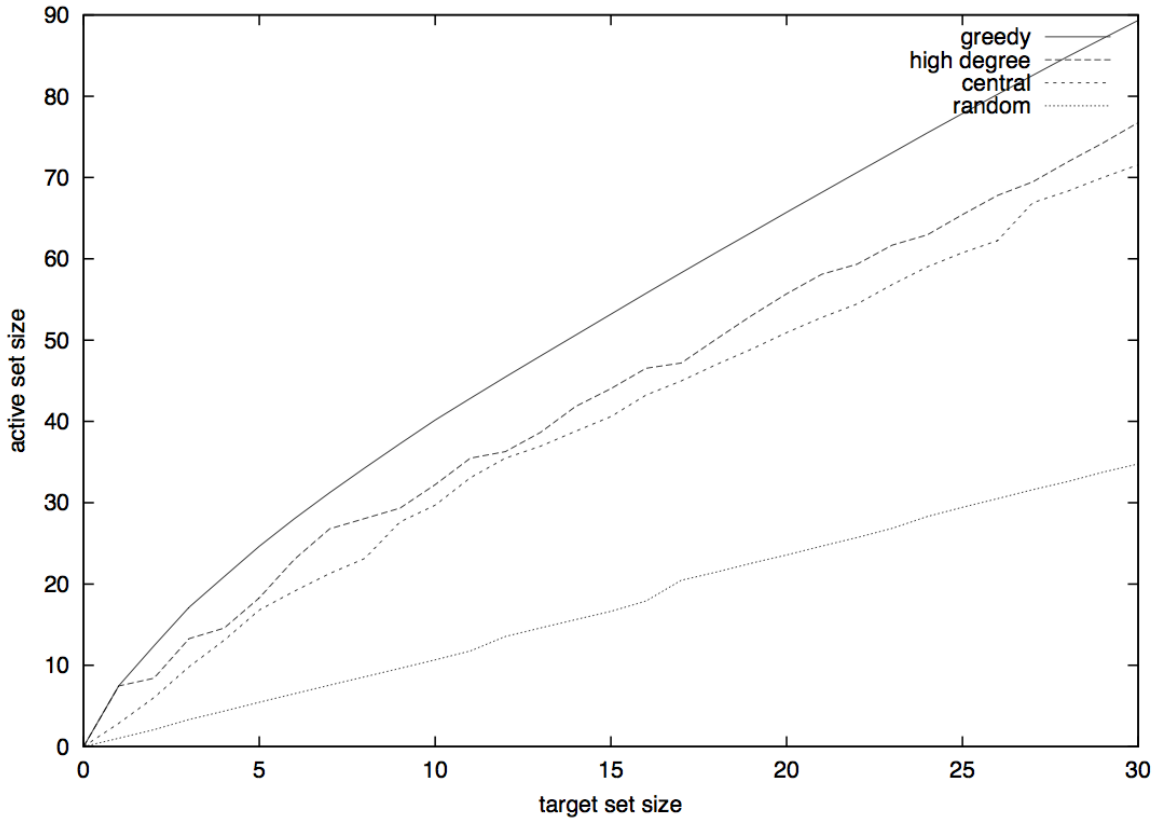

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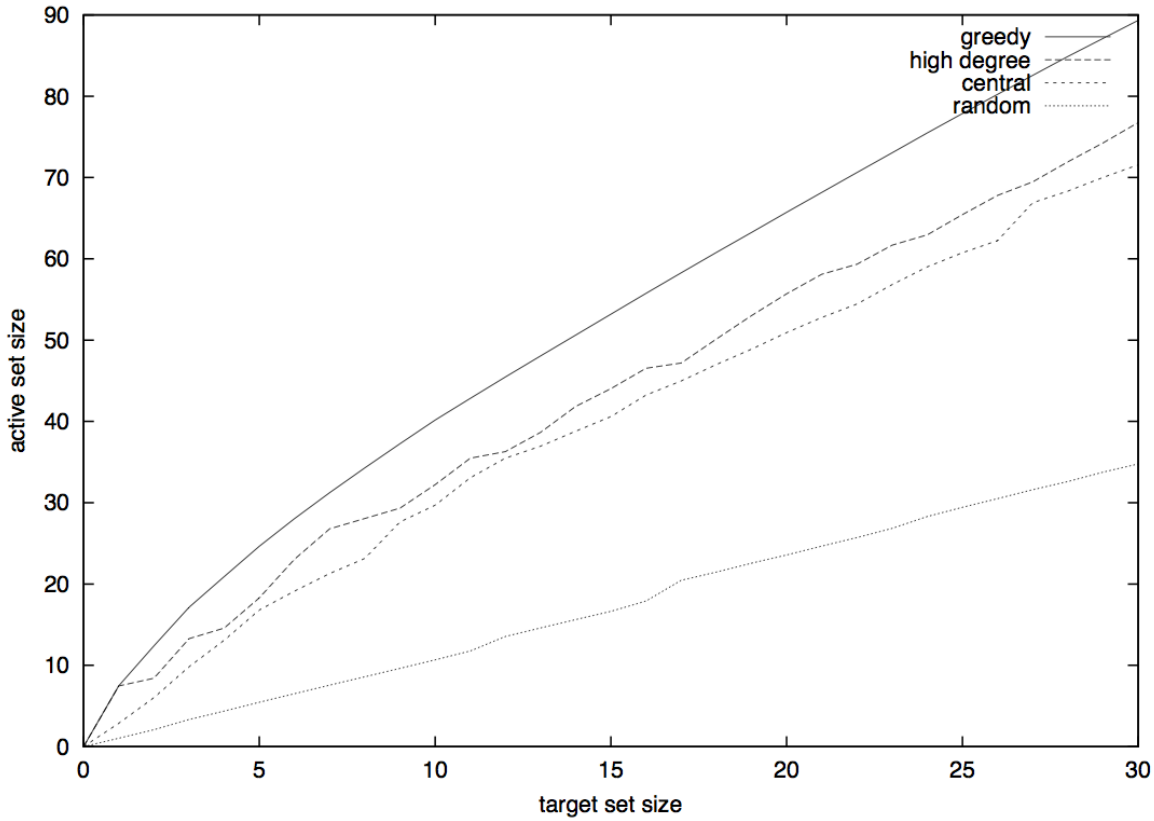

greedy approximation does better than the centrality measures

Natural graphs from utility and technology networks

- power grids, roads, Internet, sensor networks

Berkeley's Floating Sensor Network

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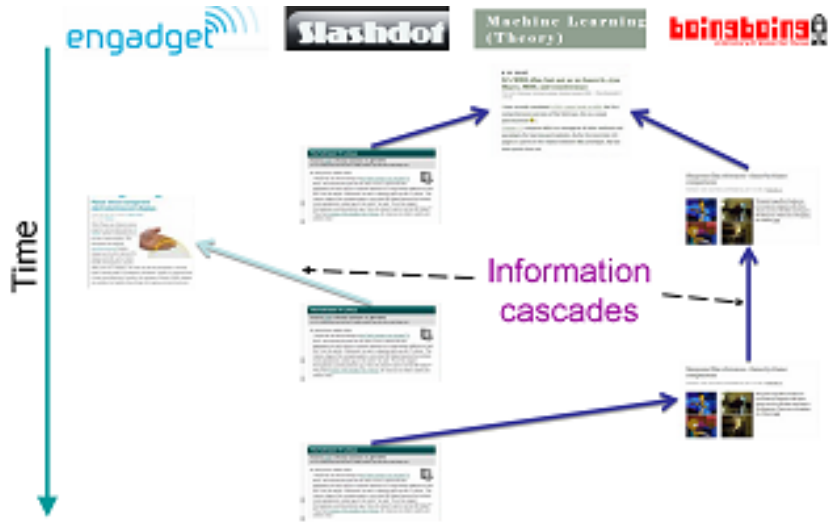
Berkeley's Floating Sensor Network

Natural graphs from information networks

- web
- blogs
- wikipedia
- typical ML tasks
  - find influential sources
  - search (`PageRank`)



Blog cascades (ETH) - *submodularity*

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Objective: **Rank** all web pages (nodes on the graph) by how **many** other pages link to them and how **important** they are.

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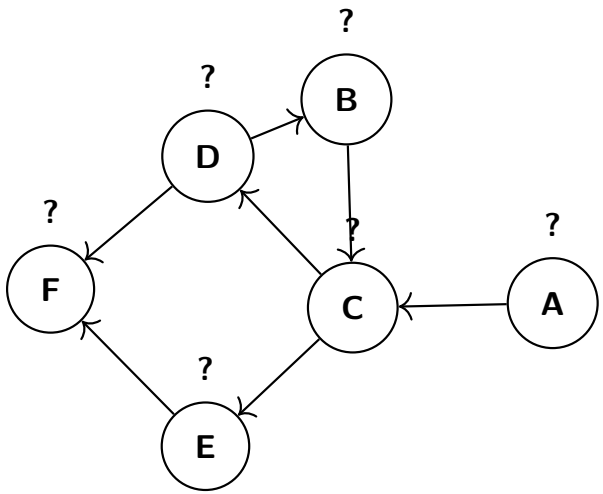

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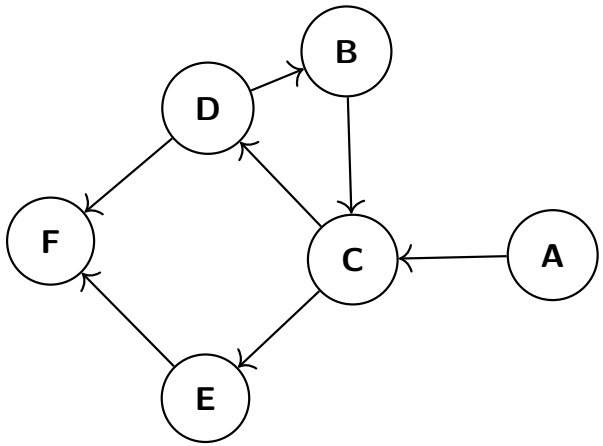

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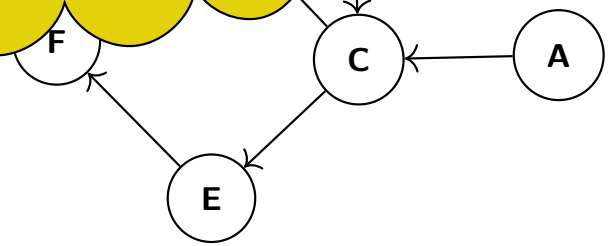

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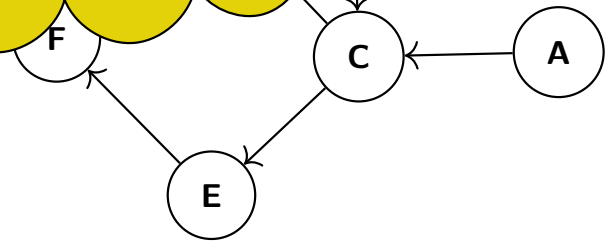

dangling pages act like sinks

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`http://infolab.stanford.edu/~backrub/google.html`:

PageRank can be thought of as a model of user behavior. We assume there is a "random surfer" who is given a web page at random and keeps clicking on links, never hitting "back" but eventually gets bored and starts on another random page.

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Google matrix: $\mathbf{G} = (1-p)\mathbf{M} + p \cdot \frac{1}{N}\mathbb{1}_{N\times N}$, where $p = 0.15$

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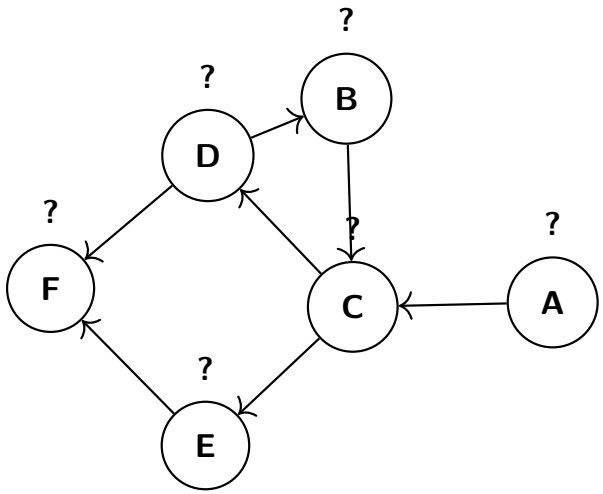

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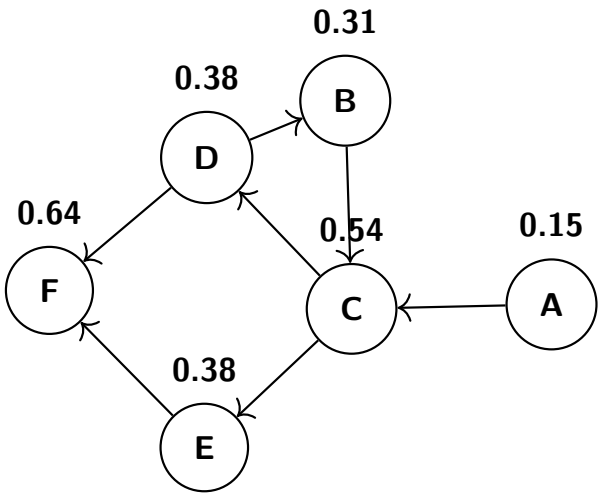

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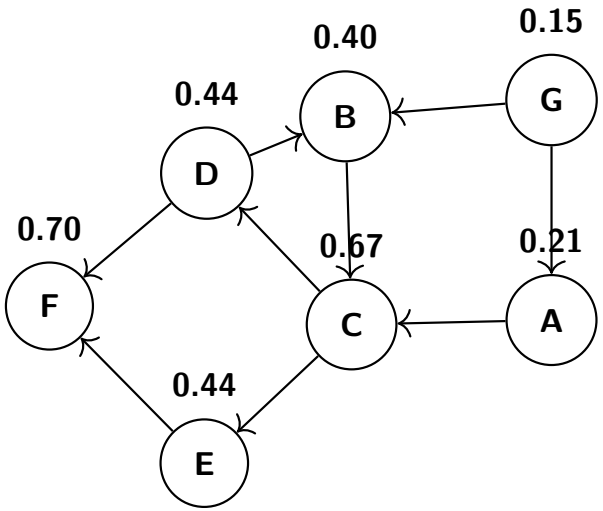

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- All search engines combined process more than 500 million queries per day

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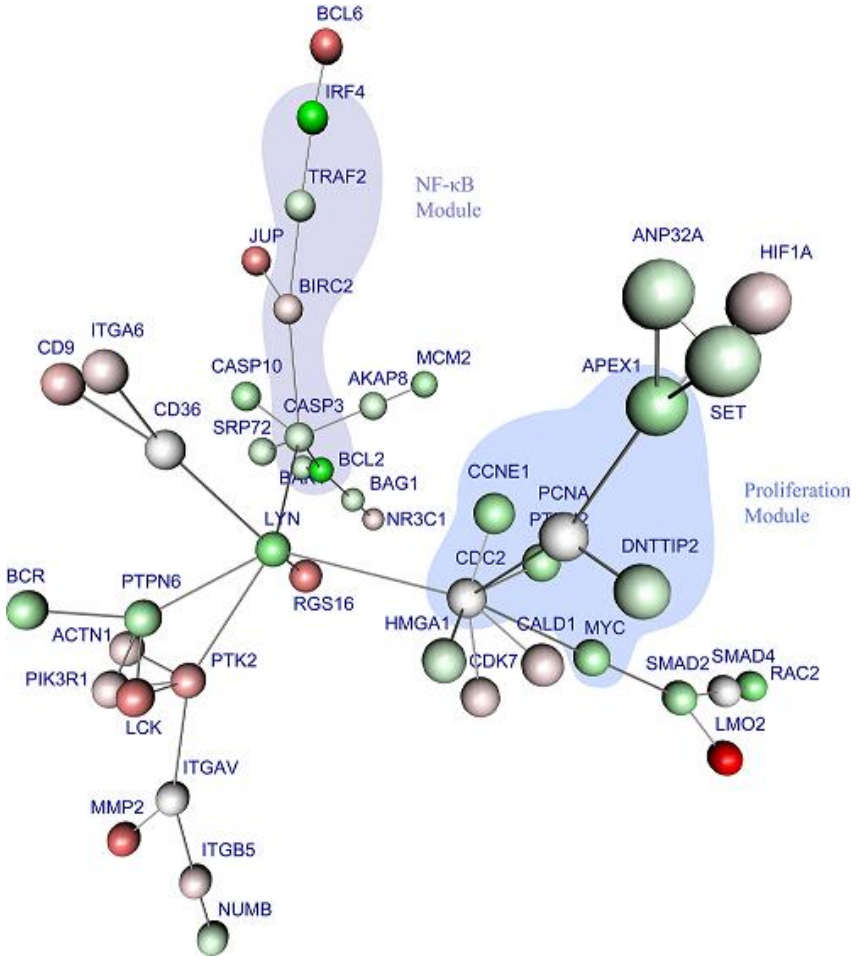
Natural graphs from biological networks

- protein-protein interactions
- gene regulatory networks
- typical ML tasks
  - discover unexplored interactions
  - learn or reconstruct the structure



Diffuse large B-cell lymphomas - Dittrich et al. (2008)

Sources of Real Networks

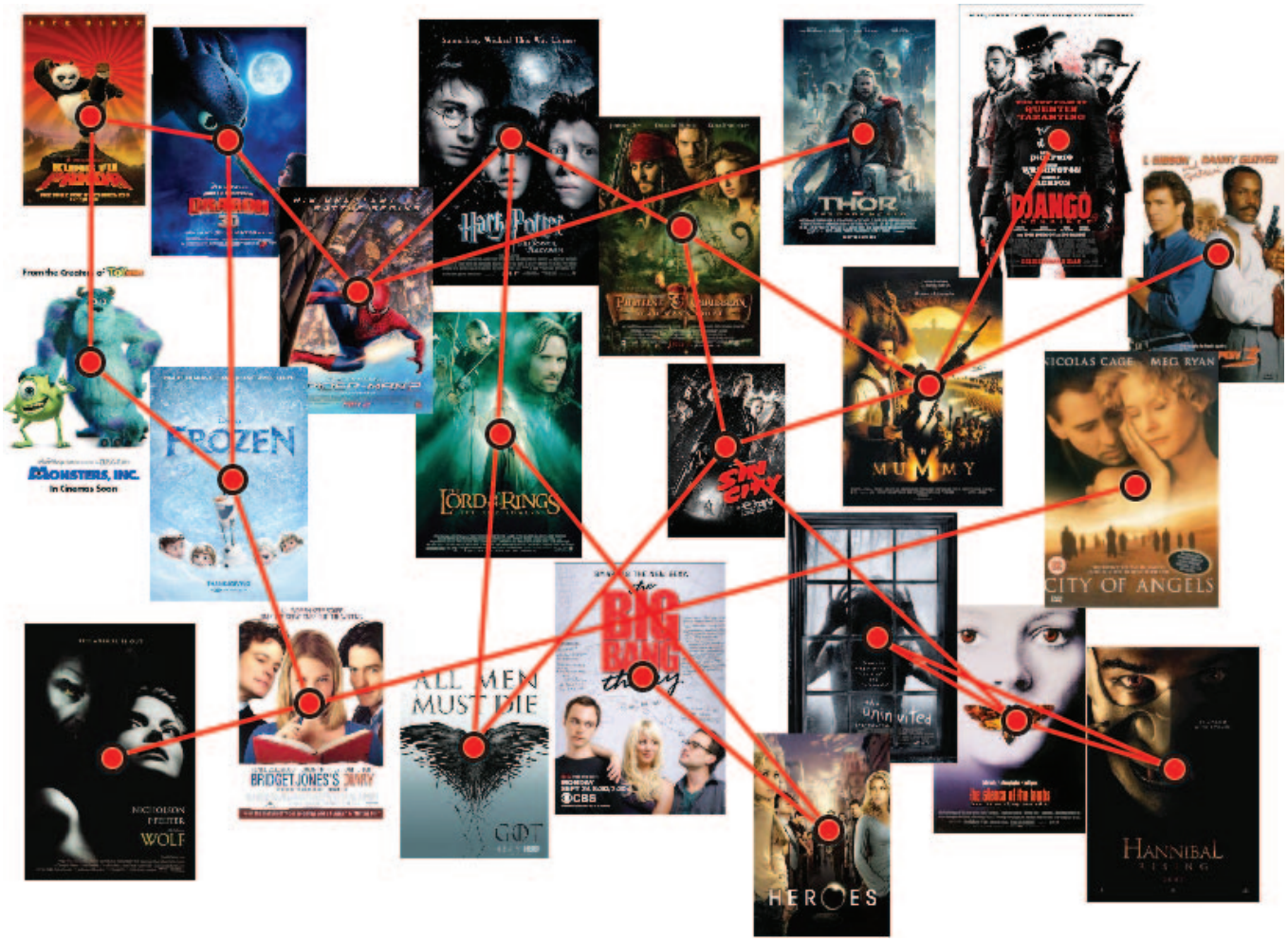
- https://ogb.stanford.edu/
- http://snap.stanford.edu/data/
- http://www-personal.umich.edu/~mejn/netdata/
- http://proj.ise.bgu.ac.il/sns/datasets.html
- http://www.cise.ufl.edu/research/sparse/matrices/
- http://vlado.fmf.uni-lj.si/pub/networks/data/default.htm

Constructed graphs from similarity networks

graph is not naturally given

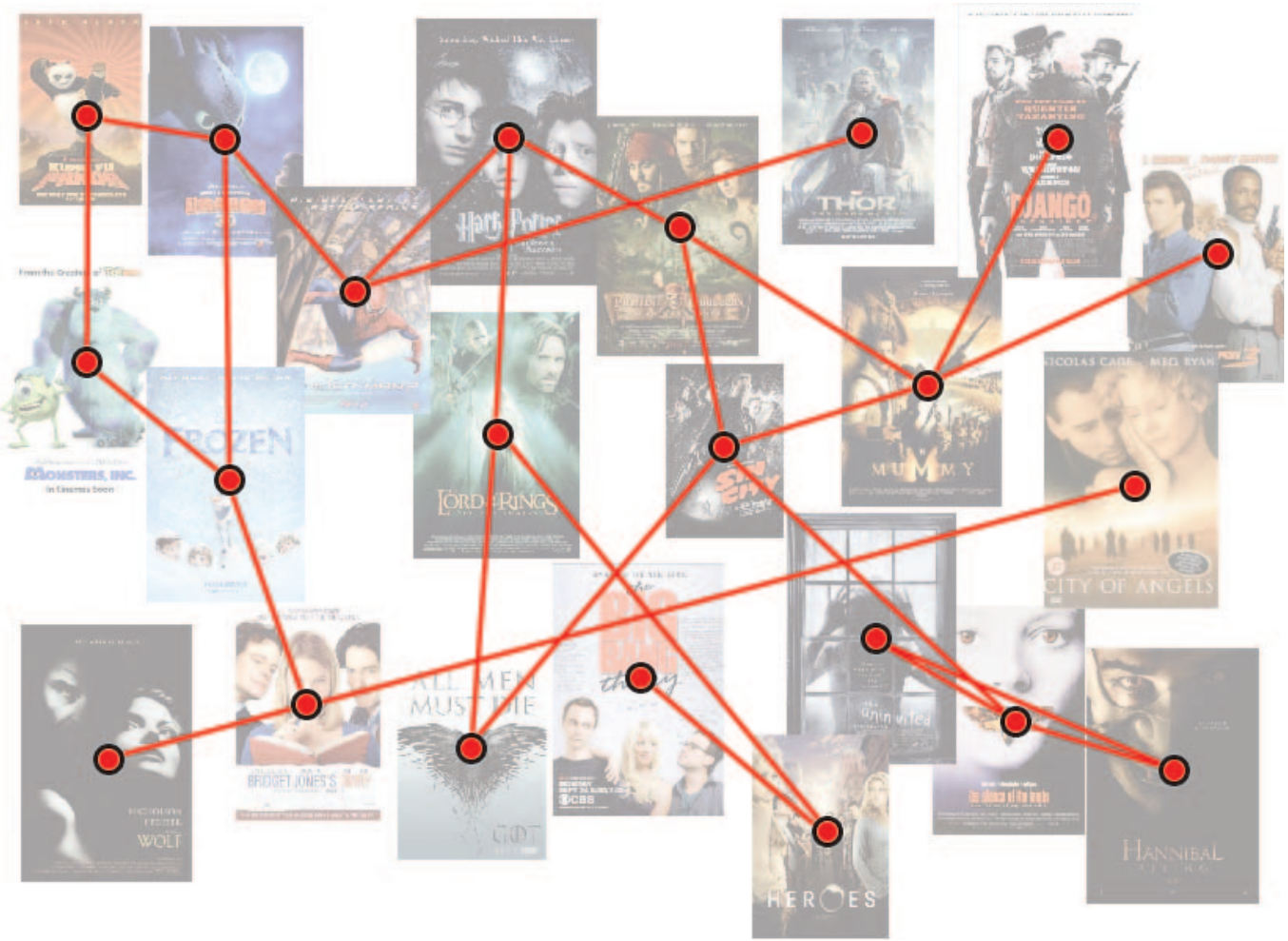
Constructed graphs from similarity networks

but we can construct it



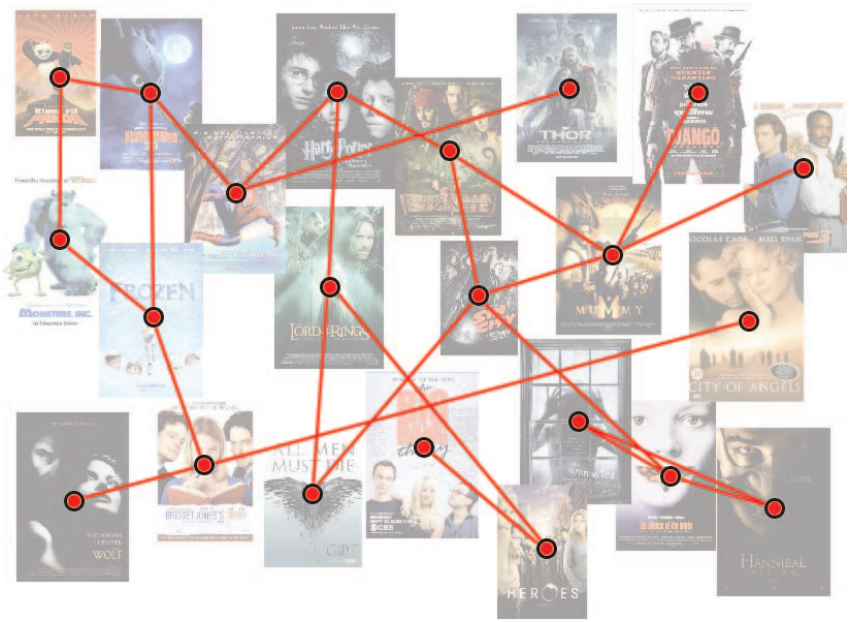
Constructed graphs from similarity networks

and use it as an abstraction



Constructed graphs from similarity networks

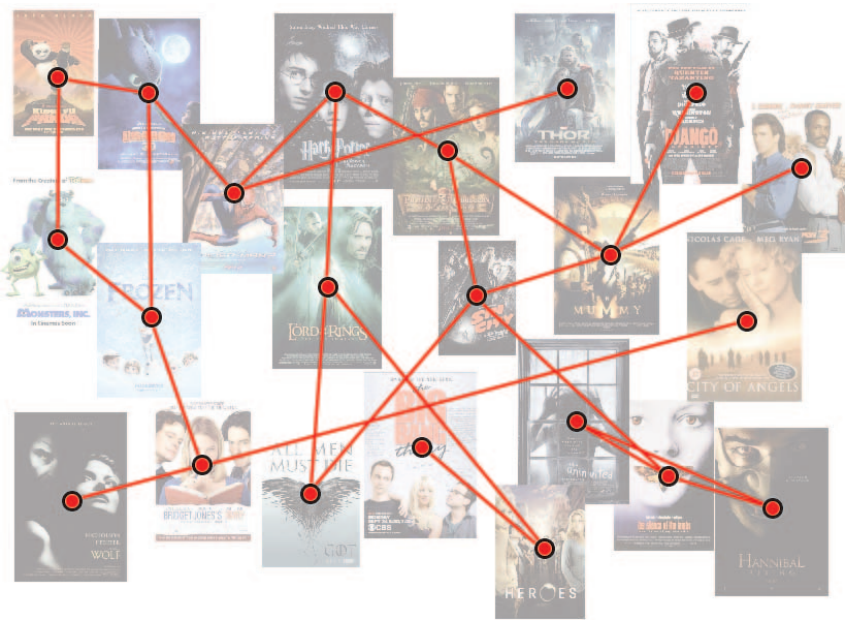
- vision
- audio
- text



movie similarity

Constructed graphs from similarity networks

- vision
- audio
- text
- typical ML tasks
  - **semi-supervised learning**
  - **spectral clustering**
  - **manifold learning**

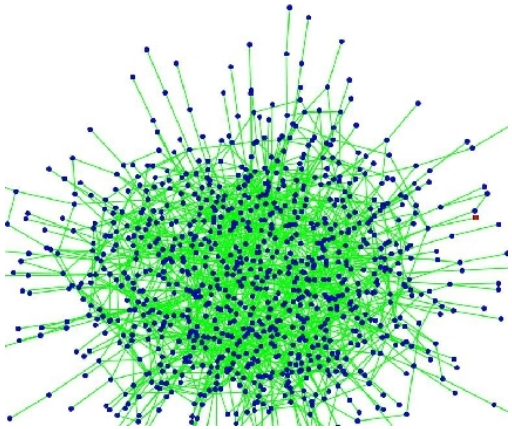


movie similarity

The in-between option: random graph models

Erdős-Rényi

independent edges



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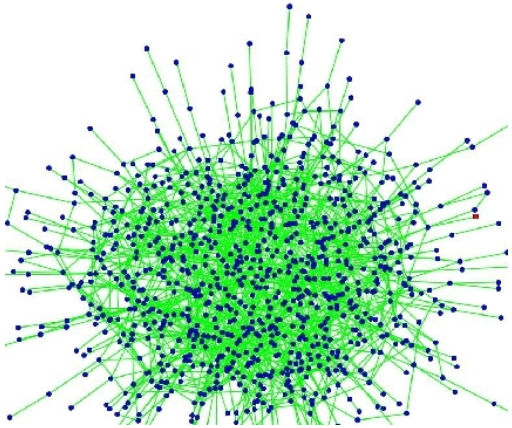
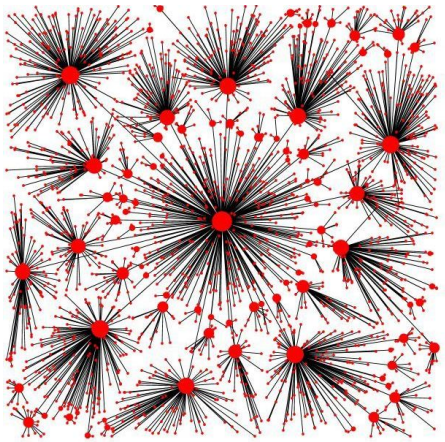


Barabási-Albert

preferential attachment



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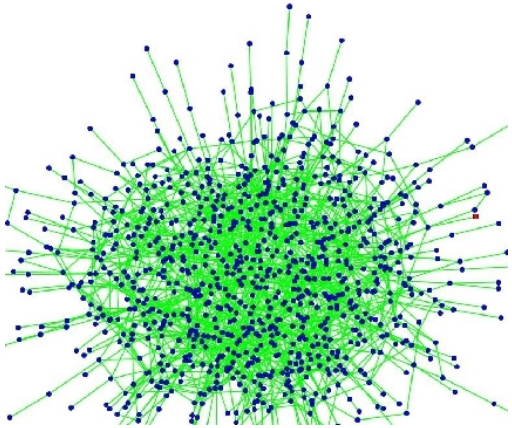

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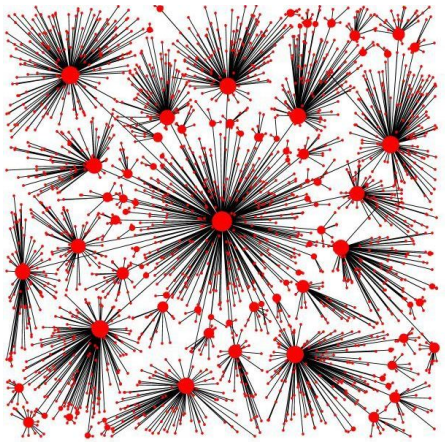

Stochastic Blocks

modeling communities

The in-between option: random graph models

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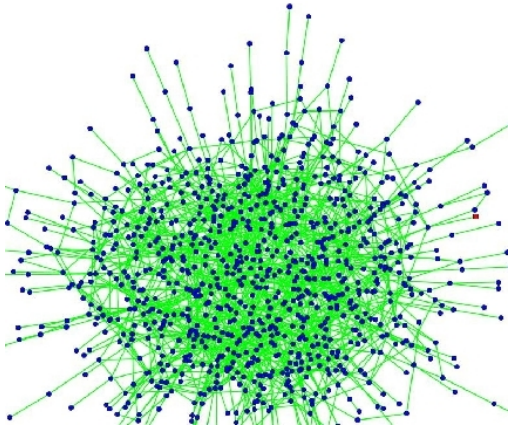

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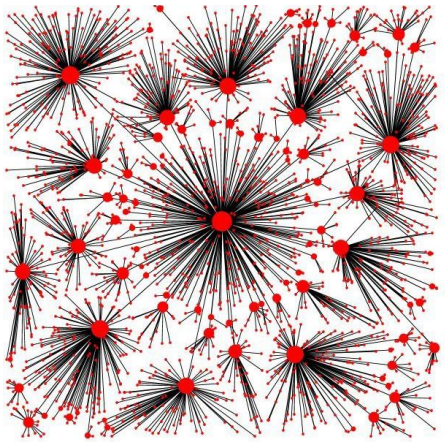
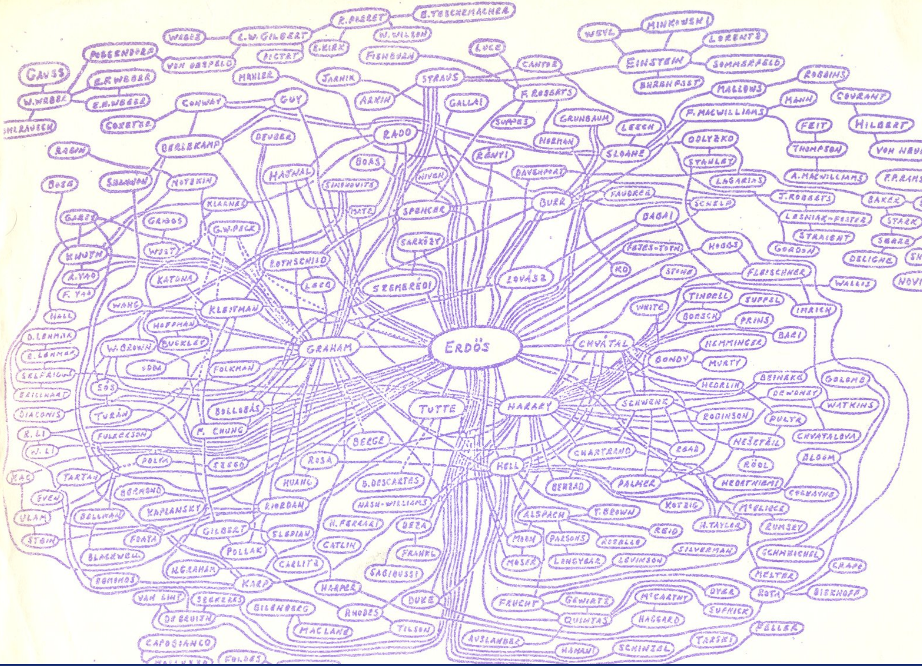


Stochastic Blocks
modeling communities

Watts-Strogatz, Chung-Lu, Fiedler, ...



Ron Graham (alias Tom Odda).

Erdős number project

- http://www.oakland.edu/enp/ try it!

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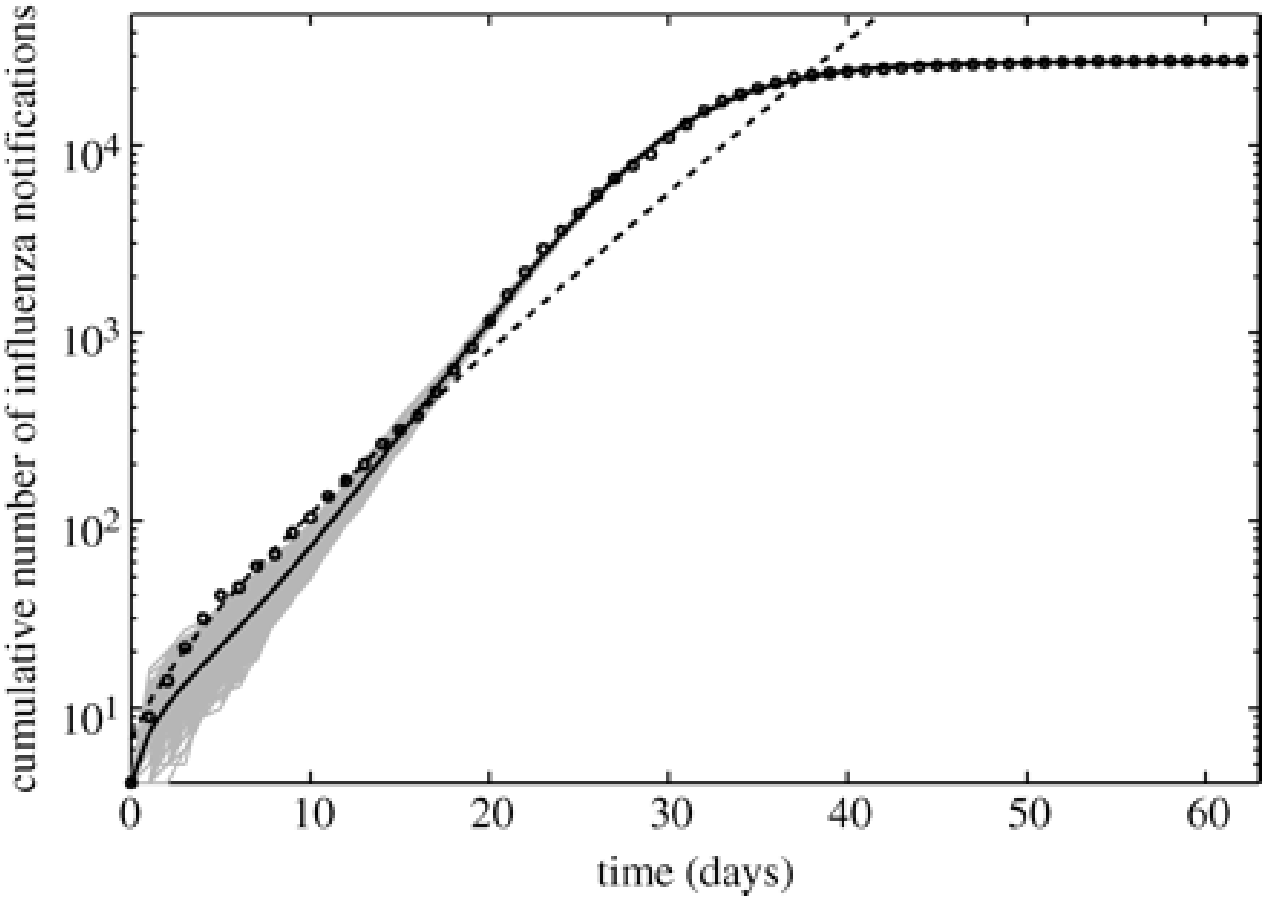
Spanish flu in San Francisco 1918–1919

Small-world phenomenon and diseases



http://rsif.royalsocietypublishing.org/content/4/12/155

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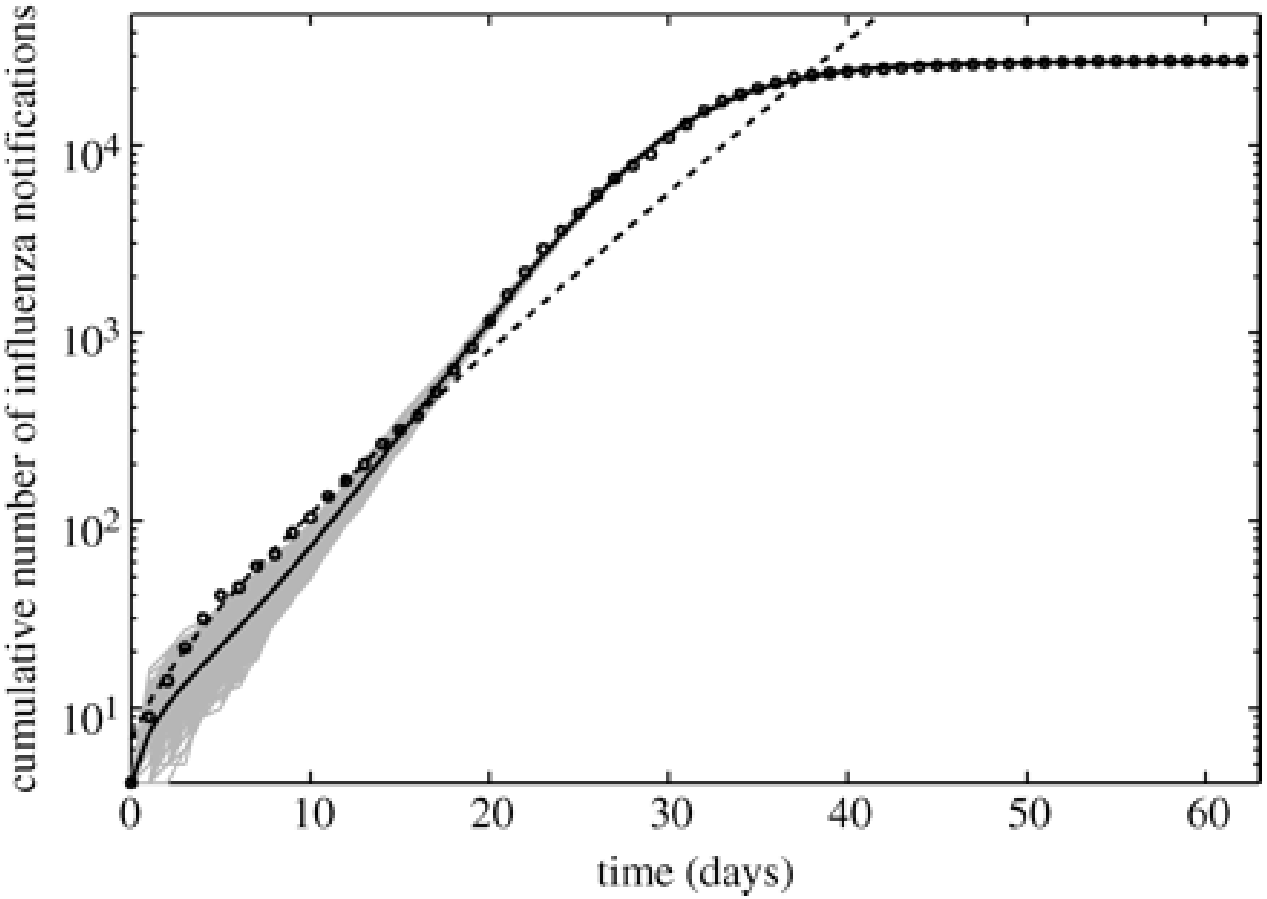
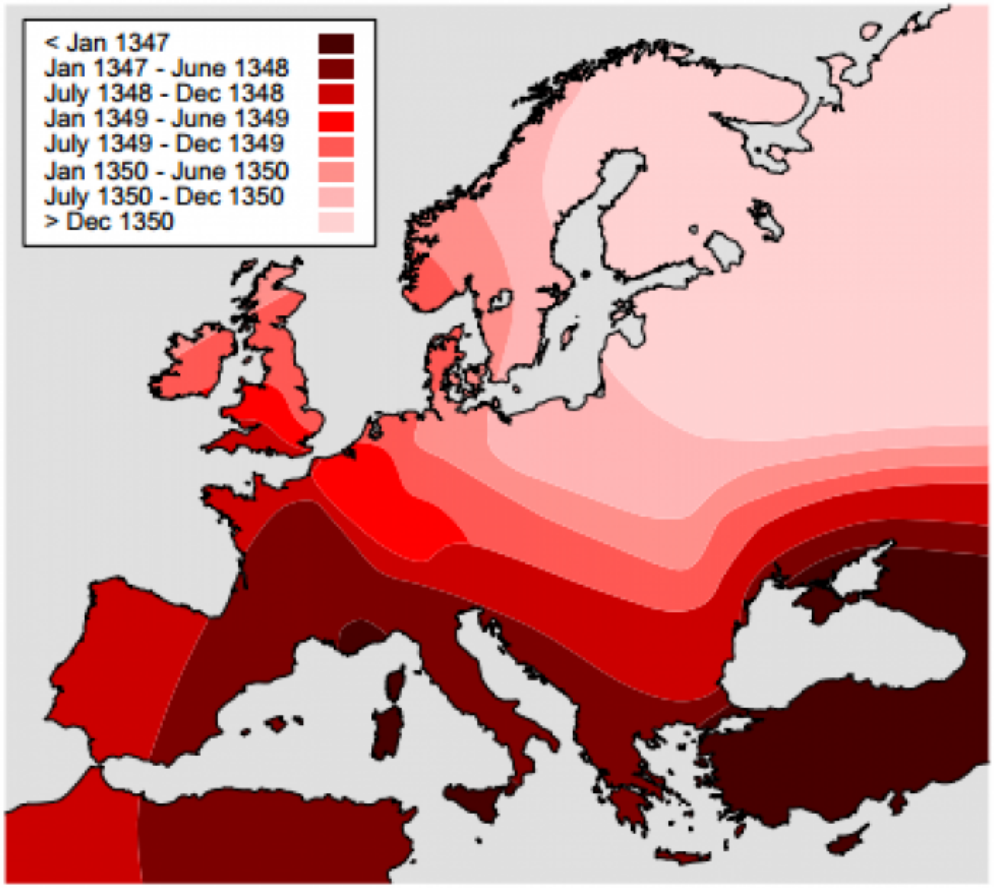


http://rsif.royalsocietypublishing.org/content/4/12/155

Small world: Obvious?

Black death!

Black death: spread



source: catholic.org

https://www.youtube.com/watch?v=EEK6c9Bh5CQ

What will you learn in the Graphs in ML course?

Concepts

What will you learn in the Graphs in ML course?

Concepts, tools

What will you learn in the Graphs in ML course?

Concepts, tools, and methods

What will you learn in the Graphs in ML course?

Concepts, tools, and methods to work with graphs in ML.

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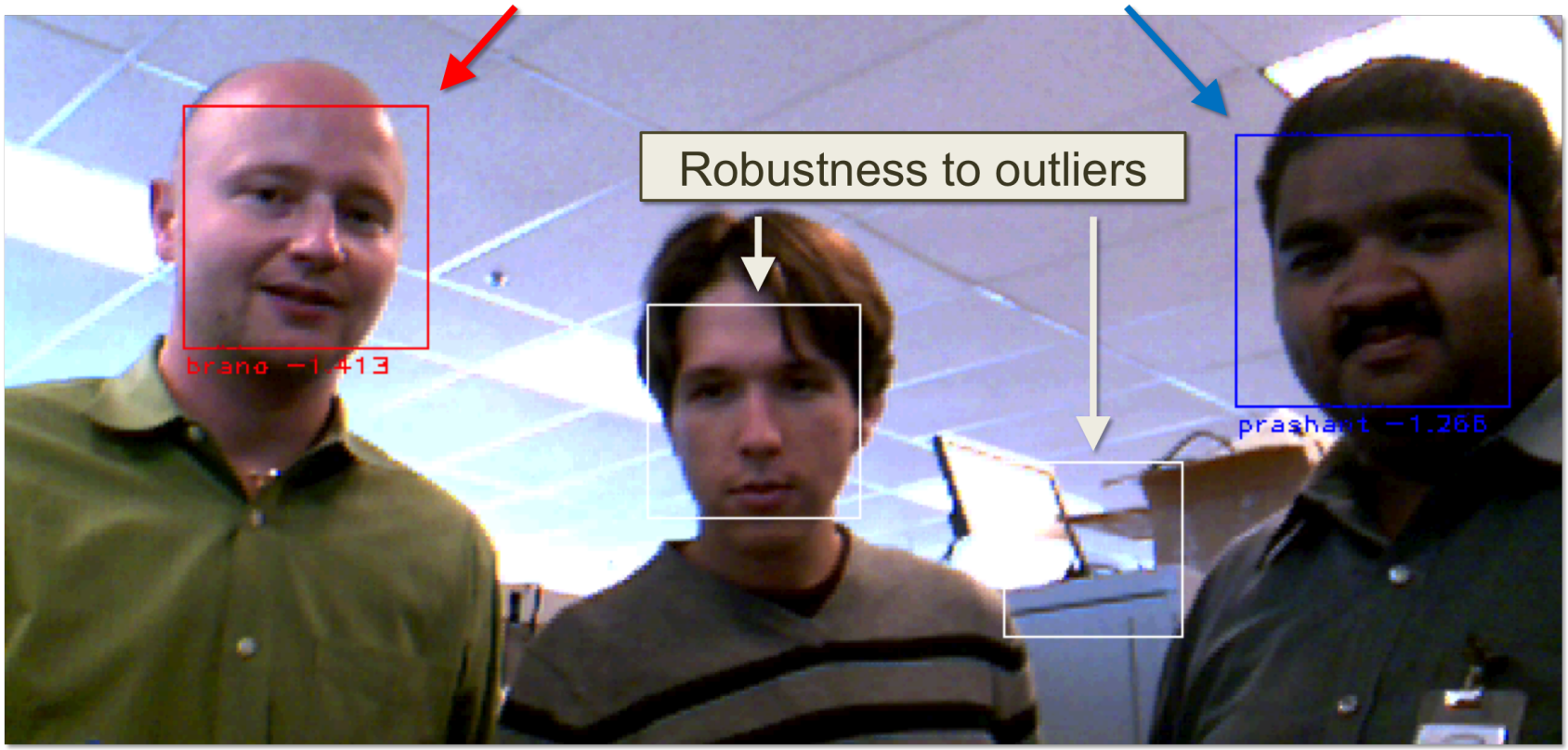
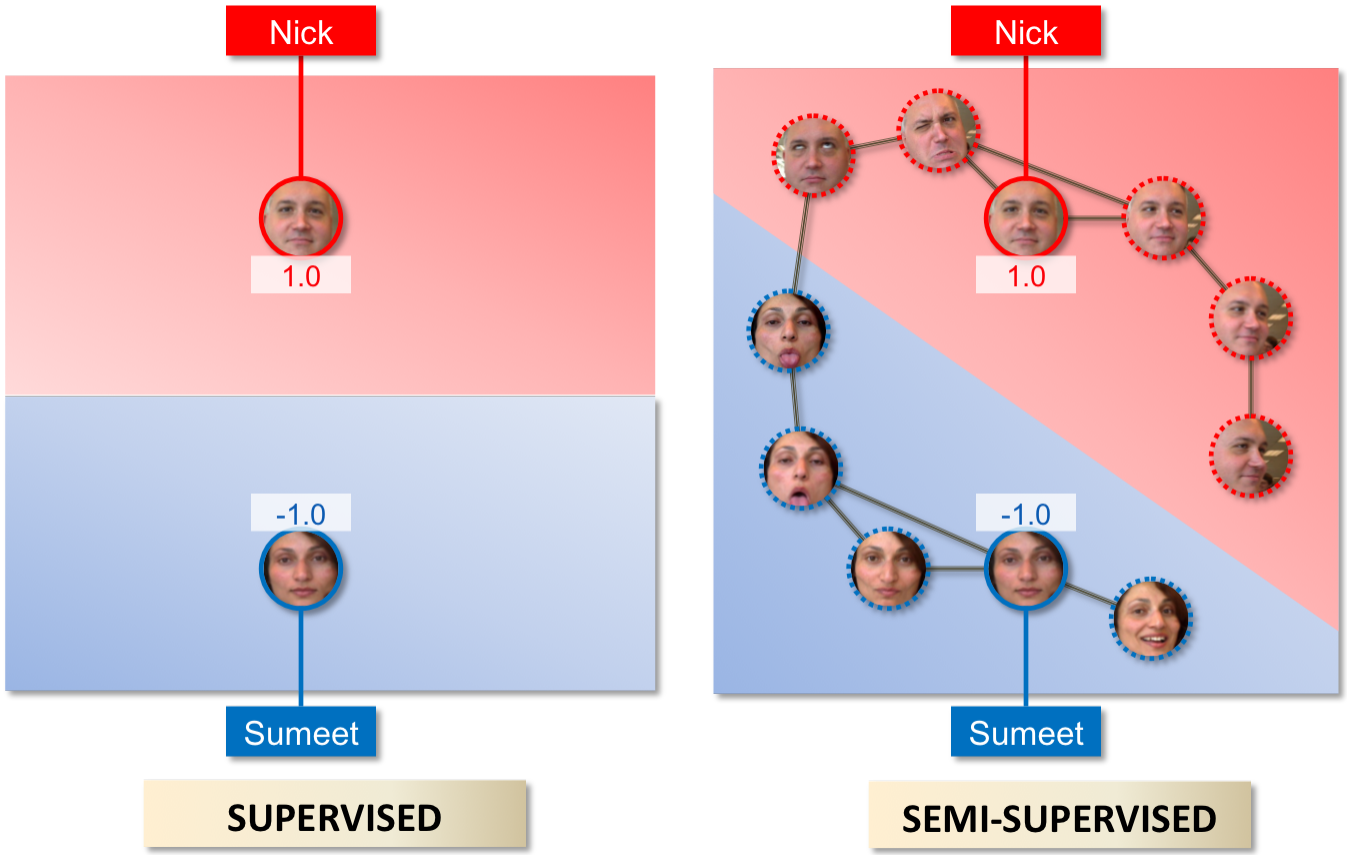
One example: Online Semi-Supervised Face Recognition

Online Semi-Supervised Face Recognition



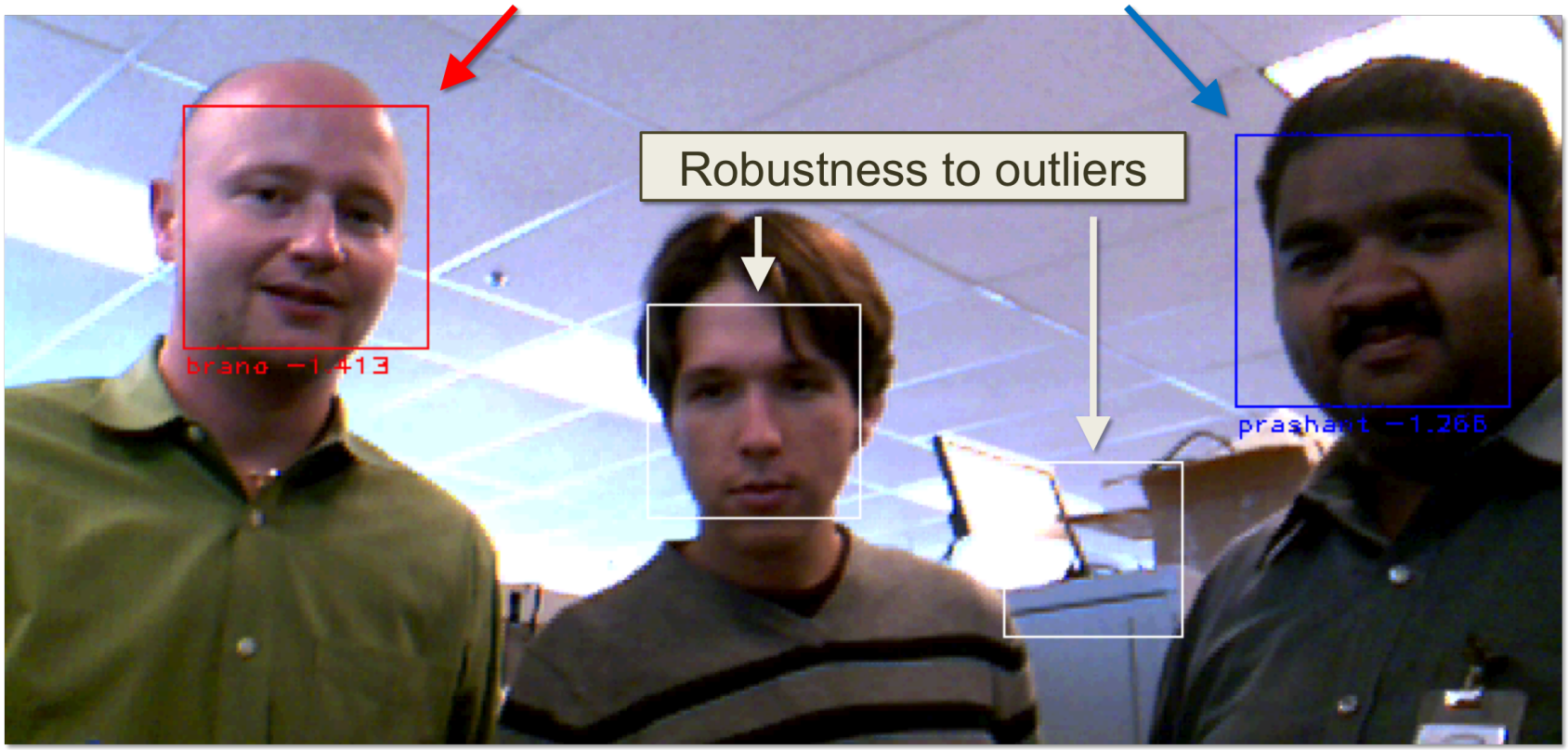
Online Semi-Supervised Face Recognition

graph-based semi-supervised learning



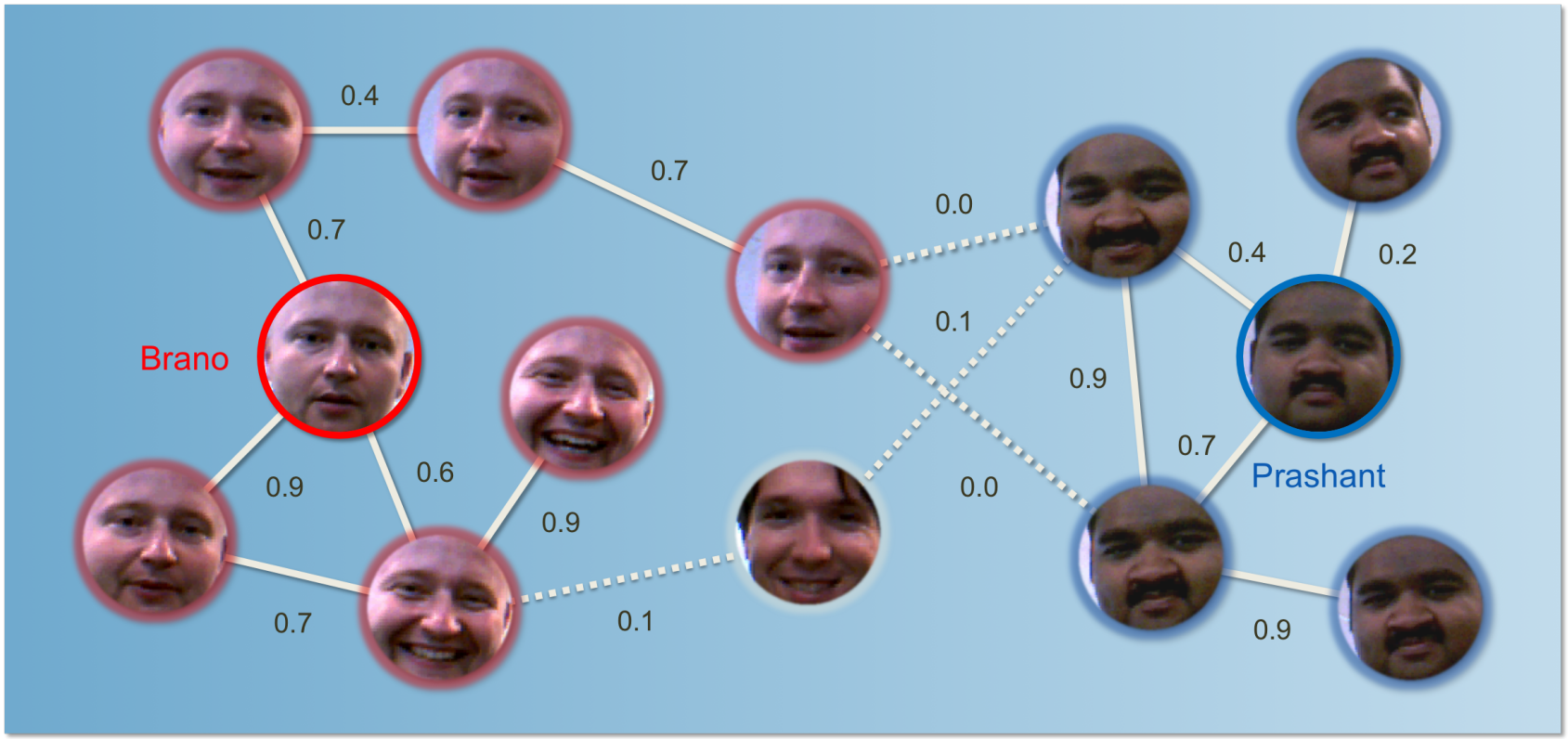
Online Semi-Supervised Face Recognition

graph is not given



Online Semi-Supervised Face Recognition

we will construct it!

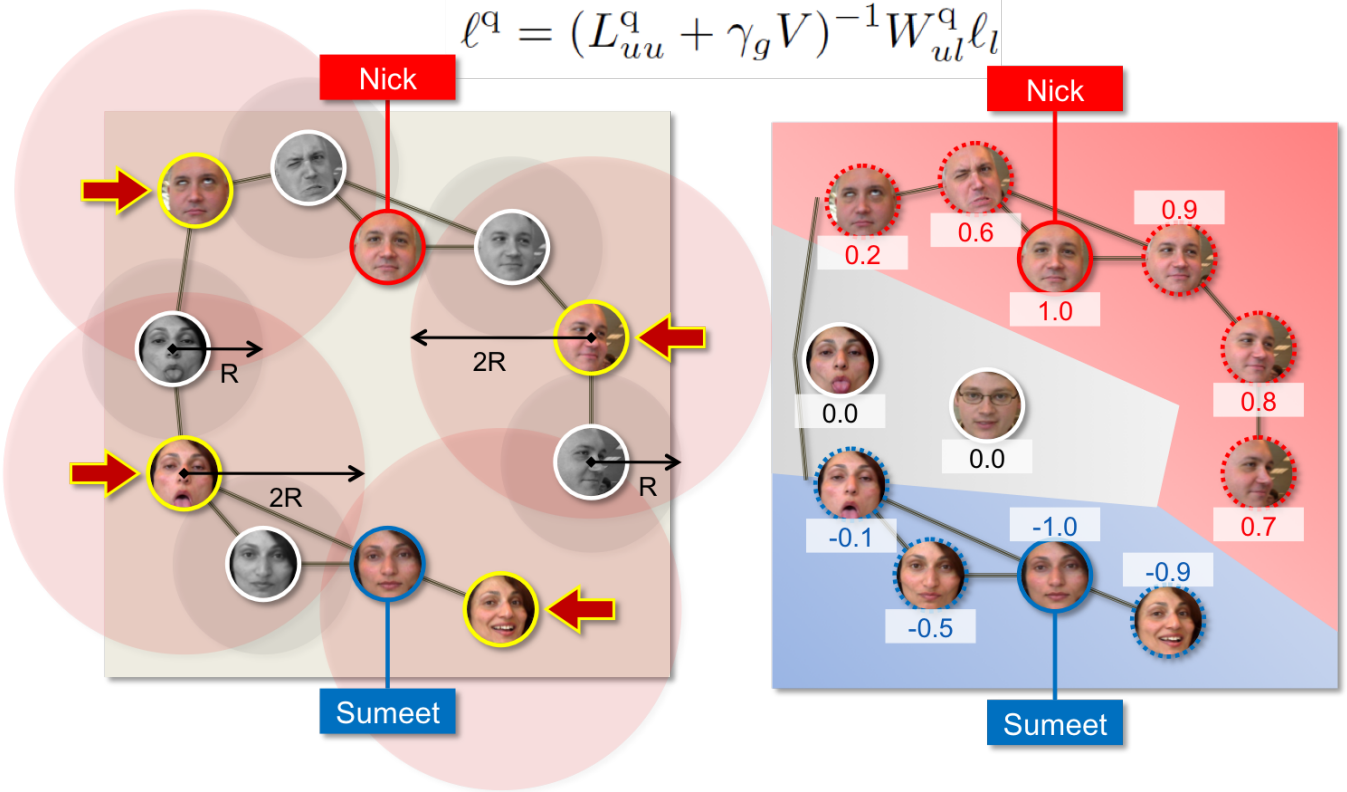


An example of a similarity graph over faces. The faces are vertices of the graph. The edges of the graph connect similar faces. Labeled faces are outlined by thick solid lines.

Online Semi-Supervised Face Recognition

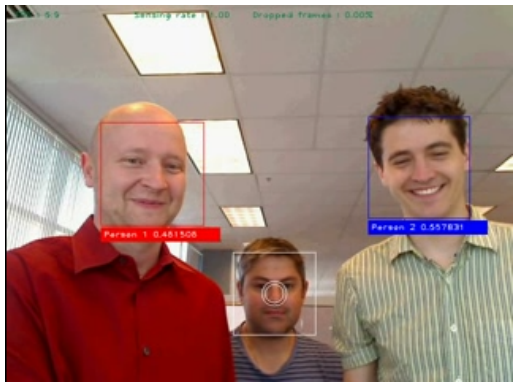
online learning - graph sparsification

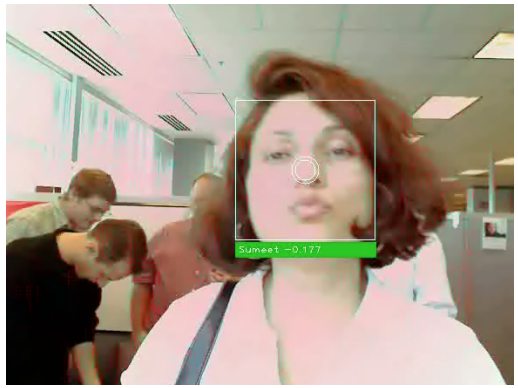
$$\ell^{\mathrm{q}} = (L^{\mathrm{q}}_{uu} + \gamma_g V)^{-1} W^{\mathrm{q}}_{ul} \ell_l$$



DEMO

second TD





see the demo: `http://researchers.lille.inria.fr/~valko/hp/serve.php?what=publications/kveton2009nipsdemo.officespace.mov`

OSS FaceReco: Analysis

$$\frac{1}{n}\sum_t (\ell_t^q[t]-y_t)^2 \le \frac{3}{n}\sum_t (\ell_t^*-y_t)^2 + \frac{3}{n}\sum_t (\ell_t^o[t]-\ell_t^*)^2 + \frac{3}{n}\sum_t (\ell_t^q[t]-\ell_t^o[t])^2$$

Error of our solution | Offline learning error | Online learning error | Quantization error

Claim: When the regularization parameter is set as $\gamma_g = \Omega(n_l^{3/2})$, the difference between the risks on labeled and all vertices decreases at the rate of $O(n_l^{-1/2})$ (with a high probability)

$$\frac{1}{n}\sum_t (\ell_t^*-y_t)^2 \le \frac{1}{n_l}\sum_{i\in\mathcal{L}} (\ell_i^*-y_i)^2 + \beta + \sqrt{\frac{2\ln(2/\delta)}{n_l}}\left(n_l\beta+4\right)$$

$$\beta \le \left[\frac{\sqrt{2}}{\gamma_g+1} + \sqrt{2n_l}\,\frac{1-\sqrt{c_u}}{\sqrt{c_u}}\,\frac{\lambda_M(L)+\gamma_g}{\gamma_g^2+1}\right]$$

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Error of our solution	Offline learning error	Online learning error	Quantization error

Claim: When the regularization parameter is set as $\gamma_g = \Omega(n^{1/4})$, the average error between the offline and online HFS predictions decreases at the rate of $O(n^{-1/2})$

$$\frac{1}{n}\sum_t (\ell_t^o[t]-\ell_t^*)^2 \le \frac{1}{n}\sum_t \left\|\ell^o[t]-\ell^*\right\|_2^2 \le \frac{4n_l}{(\gamma_g+1)^2}$$

$$\left\|\ell\right\|_2 \le \frac{\left\|y\right\|_2}{\lambda_m(C^{-1}K+I)} = \frac{\left\|y\right\|_2}{\lambda_m(K)\lambda_M^{-1}(C)+1} \le \frac{\sqrt{n_l}}{\gamma_g+1}$$

OSS FaceReco: Analysis

$$\frac{1}{n}\sum_t (\ell_t^{\mathrm{q}}[t]-y_t)^2 \le \frac{3}{n}\sum_t (\ell_t^{*}-y_t)^2 + \frac{3}{n}\sum_t (\ell_t^{\mathrm{o}}[t]-\ell_t^{*})^2 + \frac{3}{n}\sum_t (\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t])^2$$

Error of our solution	Offline learning error	Online learning error	Quantization error

Claim: When the regularization parameter is set as $\gamma_g = \Omega(n^{1/8})$, and the Laplacians L^{q} and L^{o} and normalized, the average error between the online and online quantized HFS predictions decreases at the rate of $O(n^{-1/2})$

$$\frac{1}{n}\sum_t (\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t])^2 \le \frac{1}{n}\sum_t \left\|\ell^{\mathrm{q}}[t]-\ell^{\mathrm{o}}[t]\right\|_2^2 \le \frac{n_l}{c_u^2\gamma_g^4}\left\|L^{\mathrm{q}}-L^{\mathrm{o}}\right\|_F^2$$

$$\left\|L^{\mathrm{q}}-L^{\mathrm{o}}\right\|_F^2 \propto O(k^{-2/d})$$

The distortion rate of online k-center clustering is $O(k^{-1/d})$, where d is dimension of the manifold and k is the number of representative vertices

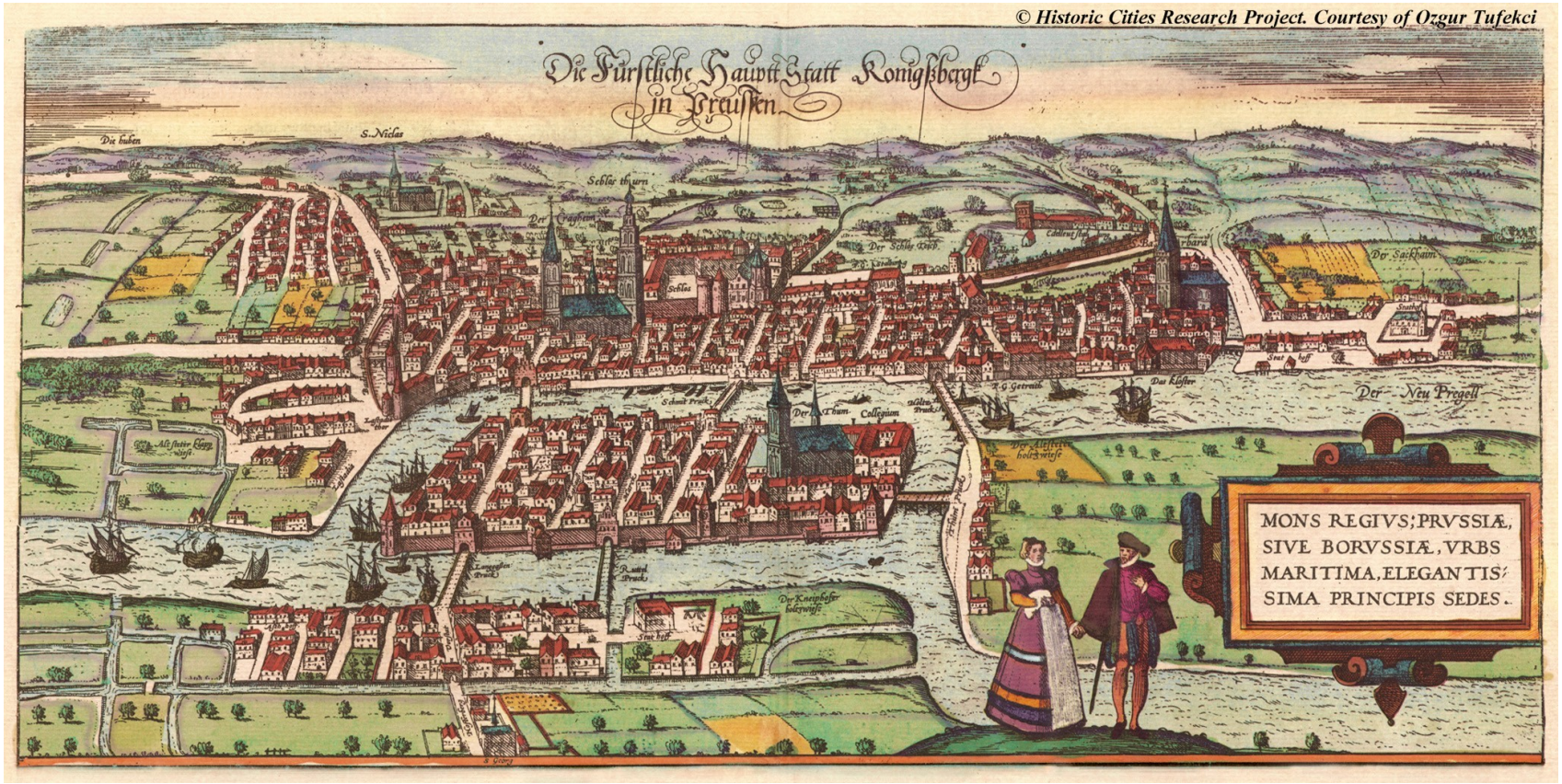
Some of the other topics

- submodularity on graphs
- graph Laplacians, spectral graph theory
- spectral clustering and manifold learning
- social network and recommender systems applications
- semi-supervised learning
- online decision-making on graphs
- learnability on graphs - transductive learning
- generalization bounds by perturbation analysis
- graph neural networks
- graph bandits
- real-world graphs scalability, spectral sparsification

Links to the other courses

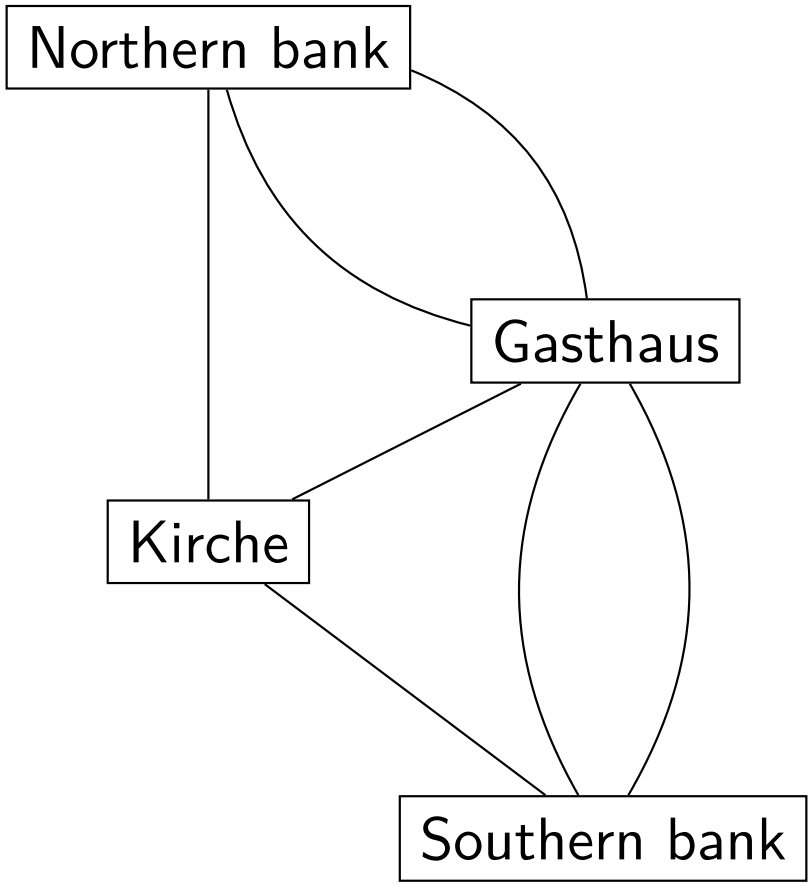
- **Introduction to statistical learning**
  - links to the learning theory on graphs: label propagation, learnability, generalization
- **Reinforcement learning**
  - link to the online learning (bandit) lecture at the end of the semester
- **Advanced learning for text and graph data**
  - data-mining graph course on the topics not covered in this course
  - details on the next slide

Graph theory refresher



Seven bridges of Konigsberg.

Graph theory refresher



Similarity Graphs

Input: $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_N$

- raw data
- flat data
- vectorial data

Similarity Graphs

Similarity graph: $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ — **(un)weighted**

Task 1: For each pair i, j: define a **similarity function** s_{ij}

Task 2: Decide which edges to include

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ε-neighborhood graphs – connect the points with the distances smaller than ε

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This is art (not much theory exists).

`http://www.informatik.uni-hamburg.de/ML/contents/people/luxburg/publications/Luxburg07_tutorial.pdf`

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Anomalies can make ε too large.

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- how to choose k?

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- metric learning (a whole field of ML)

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