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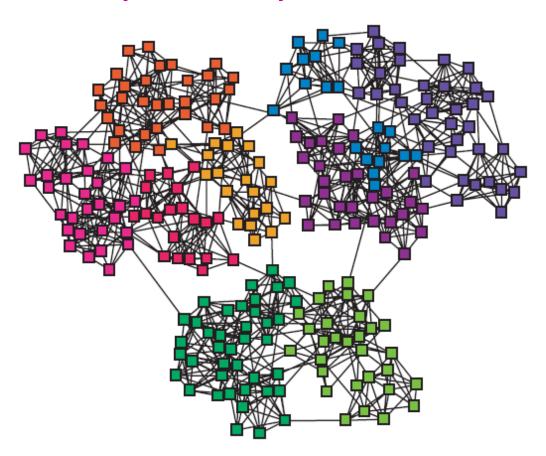
Community Detection in Graphs

CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
Charilaos Kanatsoulis, Stanford University
http://cs246.stanford.edu

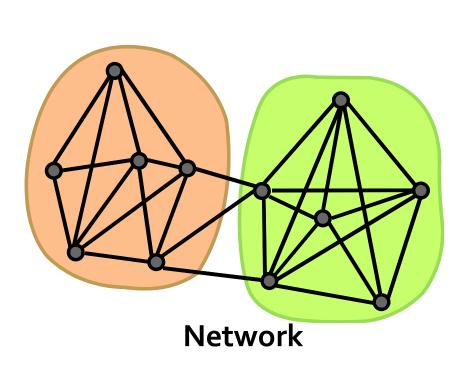


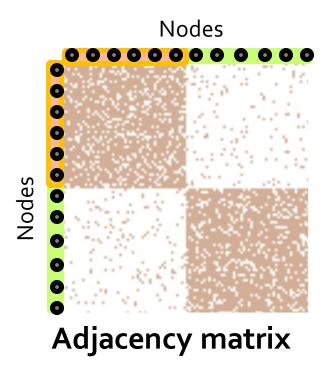
Networks & Communities

 We often think of networks being organized into modules, clusters, communities:

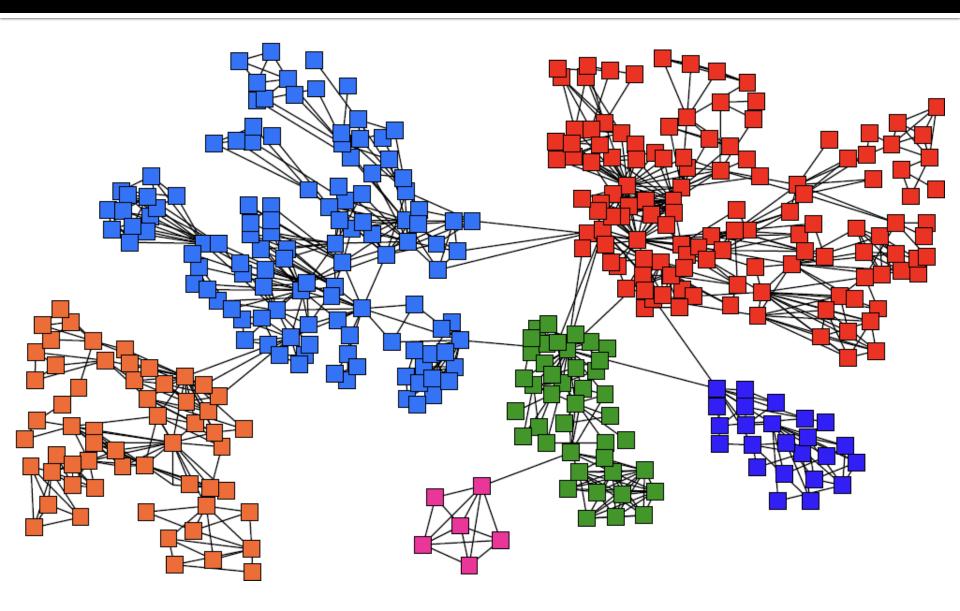


Non-overlapping Clusters



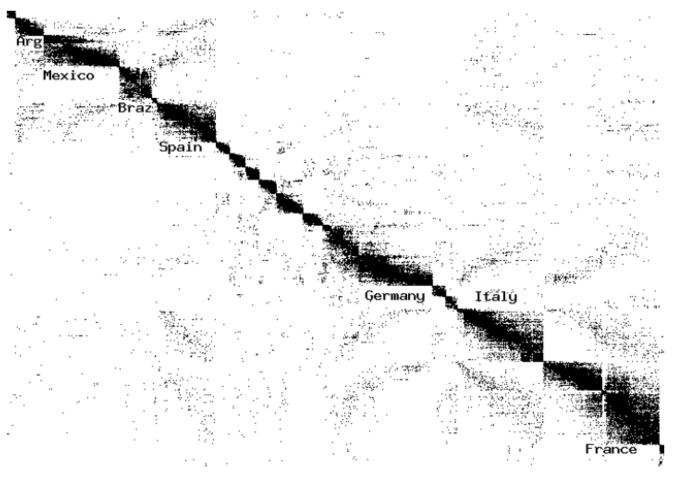


Goal: Find Densely Linked Clusters



Movies and Actors

Clusters in Movie-to-Actors Graph



[Andersen, Lang: Communities from seed sets, 2006]

Micro-Markets in Sponsored Search

Find micro-markets by partitioning the query-to-advertiser graph:



[Andersen, Lang: Communities from seed sets, 2006]

Scaling to super-large graphs: PageRank Nibble

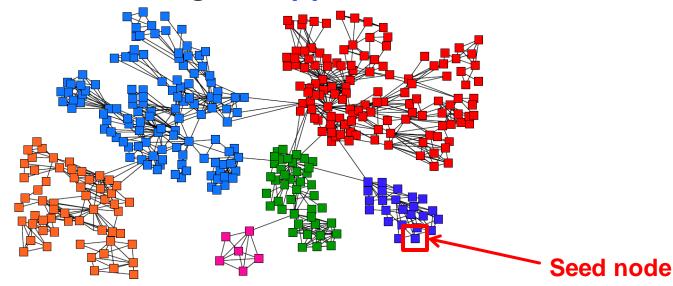
The Setting

Graph is large

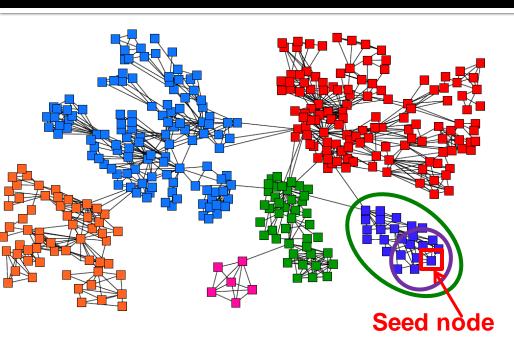
- Assume the graph fits in main memory
 - For example, to work with a 200M node and 2B edge graph one needs approx. 16GB RAM.
- But the graph is too big for running anything more than linear time algorithms.
- We will cover a PageRank based algorithm for finding dense clusters.
 - The runtime of the algorithm will be proportional to the cluster size (not the graph size!).

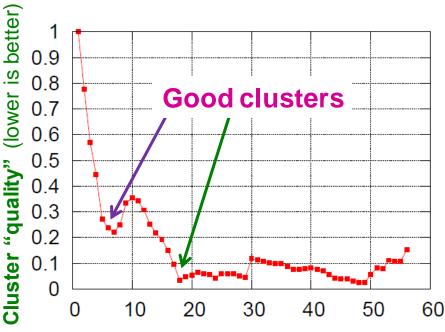
Idea: Seed Nodes

- Discovering clusters based on seed nodes
 - Given: Seed node s
 - Compute (approximate) Personalized PageRank
 (PPR) around node s (teleport set={s})
 - Idea is that if s belongs to a nice cluster, the random walk will get trapped inside the cluster



Seed Node: Intuition





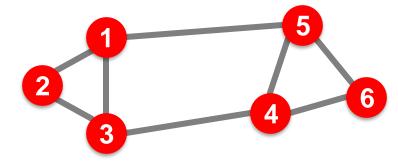
Algorithm outline:

Node rank in decreasing PPR score

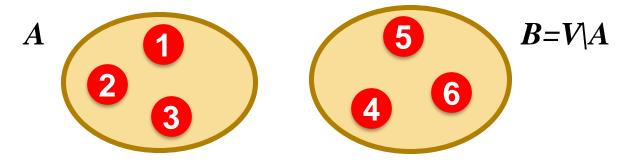
- Pick a seed node s of interest
- Run PPR with teleport set = {s}
- Sort the nodes by the decreasing PPR score
- Sweep over the nodes and find good clusters

What makes a good cluster?

• Undirected graph G(V, E):



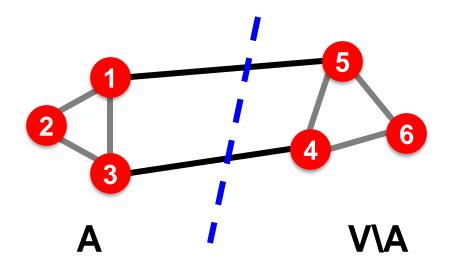
- Partitioning task:
 - Divide vertices into 2 disjoint groups $A, B = V \setminus A$



- Question:
 - How can we define a "good" cluster in G?

What makes a good cluster?

- What makes a good cluster?
 - Maximize the number of within-cluster connections
 - Minimize the number of between-cluster connections

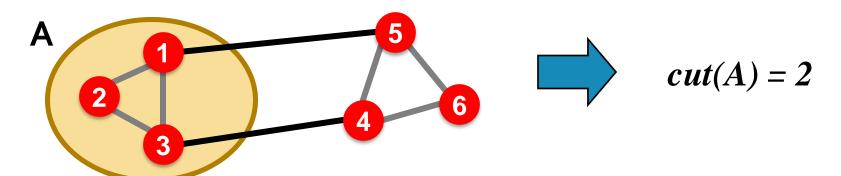


Graph Cuts

- Express cluster quality as a function of the "edge cut" of the cluster
- Cut: Set of edges (edge weights) with only one node in the cluster:

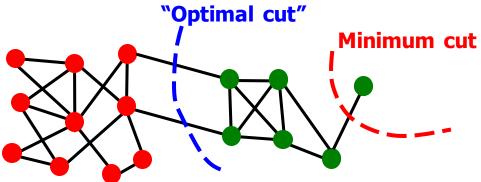
$$cut(A) = \sum_{i \in A, j \notin A} w_{ij}$$

Note: This works for weighted and unweighted (set all **w**_{ij}=1) undirected graphs



Cut Score

- Partition quality: Cut score
 - Quality of a cluster is the weight of connections pointing outside the cluster
- Not so uncommon case:



- Problem:
 - Only considers (external) inter-cluster connections
 - Does not consider (internal) intra-cluster connectivity

Graph Partitioning Criteria

Criterion: Conductance:

Connectivity of the group to the rest of the network relative to the density of the group

$$\phi(A) = \frac{|\{(i, j) \in E; i \in A, j \notin A\}|}{\min(vol(A), 2m - vol(A))}$$

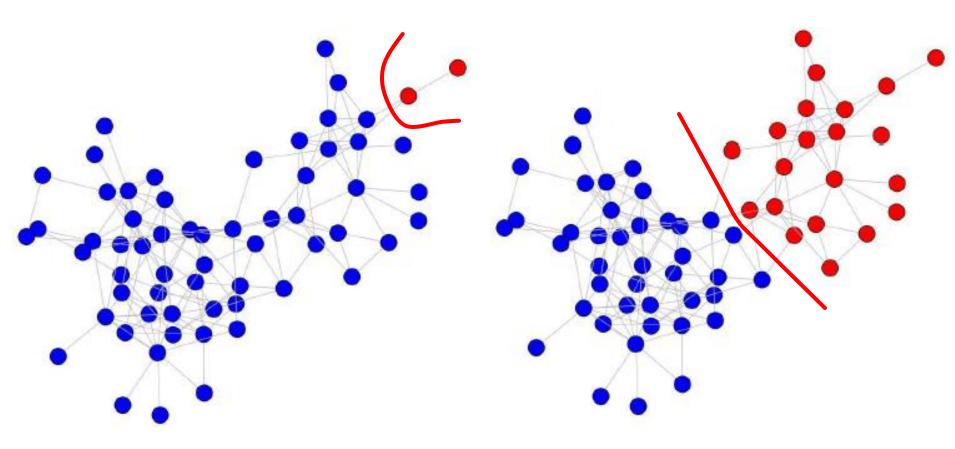
vol(A): total weight of the edges with at least one endpoint in A: $vol(A) = \sum_{i \in A} d_i$

- Vol(A)=2*#edges inside A + #edges pointing out of A
- Why use conductance?
 - Produces more balanced partitions

m... number of edges of the graph

d_i... degree of node *I*E...edge set of the graph

Example: Conductance Score



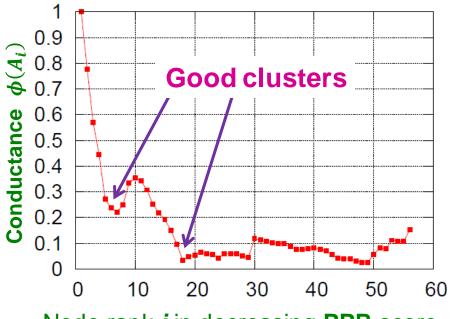
$$\phi = 2/4 = 0.5$$

$$\phi = 6/92 = 0.065$$

Algorithm Outline: Sweep

Algorithm outline:

- Pick a seed node s of interest
- Run PPR w/ teleport={s}
- Sort the nodes by the decreasing PPR score
- Sweep over the nodes and find good clusters



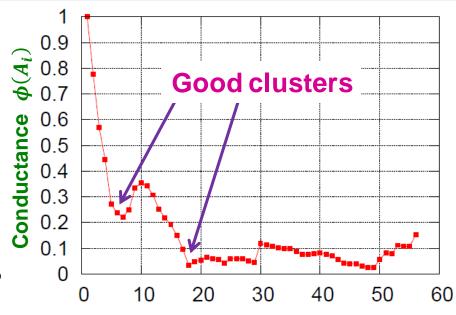
Node rank *i* in decreasing **PPR** score

Sweep:

- Sort nodes by decreasing PPR score $r_1 > r_2 > \cdots > r_n$
- For each i compute $\phi(A_i = \{u_1, ... u_i\})$
- **Local minima** of $\phi(A_i)$ correspond to good clusters

Computing the Sweep

- The whole Sweep curve can be computed in linear time:
 - For loop over the nodes
 - Keep hash-table of nodes in a set A_i



Node rank *i* in decreasing **PPR** score

- To compute $\phi(A_{i+1}) = Cut(A_{i+1})/Vol(A_{i+1})$
 - $Vol(A_{i+1}) = Vol(A_i) + d_{i+1}$
 - $Cut(A_{i+1}) = Cut(A_i) + d_{i+1} 2\#(edges\ of\ u_{i+1}\ to\ A_i)$

Computing PPR

- How to compute Personalized PageRank (PPR) without touching the whole graph?
 - Power method won't work since each single iteration

accesses all nodes of the graph:
$$\mathbf{r^{(t+1)}} = \beta \mathbf{M} \cdot \mathbf{r^{(t)}} + (\mathbf{1} - \boldsymbol{\beta})\boldsymbol{a}$$
 At index S

- a is a teleport vector: $a = [0 \dots 0 \stackrel{\bullet}{1} 0 \dots 0]^T$
- r is the personalized PageRank vector
- Approximate PageRank (AKA PageRank-Nibble) [Andersen, Chung, Lang, '07]
 - A fast method for computing approximate Personalized PageRank (PPR) with teleport set S={s}
 - ApproxPageRank(s, β, ε)
 - **s** ... seed node
 - β ... teleportation parameter
 - ε ... approximation error parameter

Approximate PPR: Overview

Approximate PPR on <u>undirected graph</u>

Lazy random walk, which is a variant of a random walk that stays put with probability 1/2 at each time step, and walks to a random neighbor the other half of the time:

$$r_u^{(t+1)} = \frac{1}{2}r_u^{(t)} + \frac{1}{2}\sum_{i \to u} \frac{1}{d_i}r_i^{(t)}$$
 $d_i \dots \text{ degree of } i$

- Keep track of <u>residual</u> PPR score $q_u = p_u r_u^{(t)}$
 - **Residual** q_u : how well is PPR score p_u of u is approximated
 - $lacktriangledown_u$ pageRank of node u
 - $r_u^{(t)}$... is PageRank estimate of node u at around t

If **residual** q_u of node u is too big $\frac{q_u}{d_u} \ge \varepsilon$ then **push the walk** further (distribute some of residual q_u to all u's neighbors along outgoing edges), else we don't touch the node

"Push" Operation

residual PPR score $q_u = p_u - r_u$

- Idea: a...teleport vector
 - r... approx. PageRank, q... its residual PageRank
 - Start with trivial approximation: r = 0 and q = a
 - Iteratively push PageRank from q to r until q is small
- Push: 1 step of a lazy random walk from node u:

```
\begin{aligned} \textit{Push}(u,r,q) \colon \\ r' &= r, \ q' = q \\ r'_u &= r_u + (1-\beta)q_u \\ q'_u &= \frac{1}{2}\beta q_u \\ \text{for each } v \text{ such that } u \to v \colon \\ q'_v &= q_v + \frac{1}{2}\beta \frac{q_u}{d_u} \\ \text{return } r', \ q' \end{aligned}
```

1-β...teleport prob

Update r
Do 1 step of a walk:
Stay at u with prob. ½
Spread remaining ½
fraction of qu as if a single step of random walk were applied to u

Intuition Behind Push Operation

Push(u,r,q):

r'=r, q'=q

 $r'_{u} = r_{u} + (1 - \beta)q_{u}$ $q'_{u} = \frac{1}{2}\beta q_{u}$

for each v such that $u \rightarrow v$:

- If q_u is large, this means that we have underestimated the importance of node u
- Then we want to take some of that residual (q_u) and give it away, since we know that we have too much of it
- So, we keep $\frac{1}{2}\beta q_u$ and then give away the rest to our neighbors, so that we can get rid of it
 - This correspond to the spreading of $\frac{1}{2}\beta q_u/d_u$ term
- Each node wants to keep giving away this excess
 PageRank until all nodes have no or a very small gap in the excess PageRank

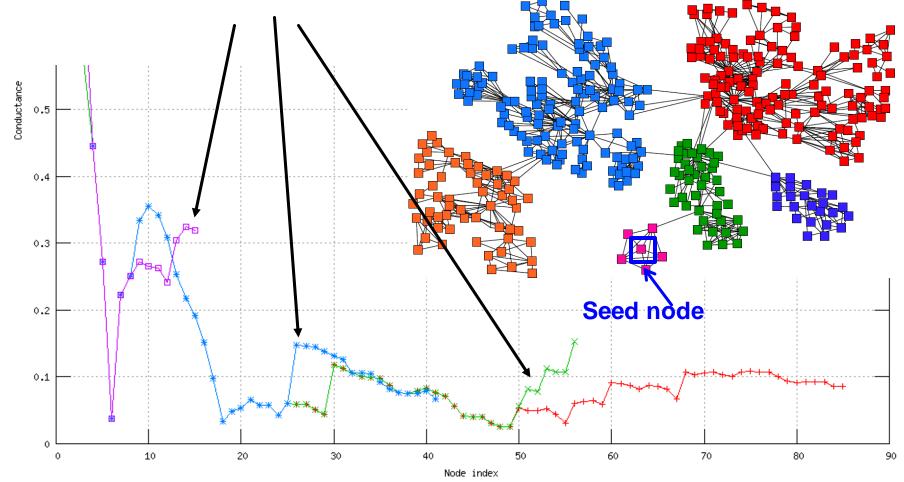
Observations (1)

Runtime:

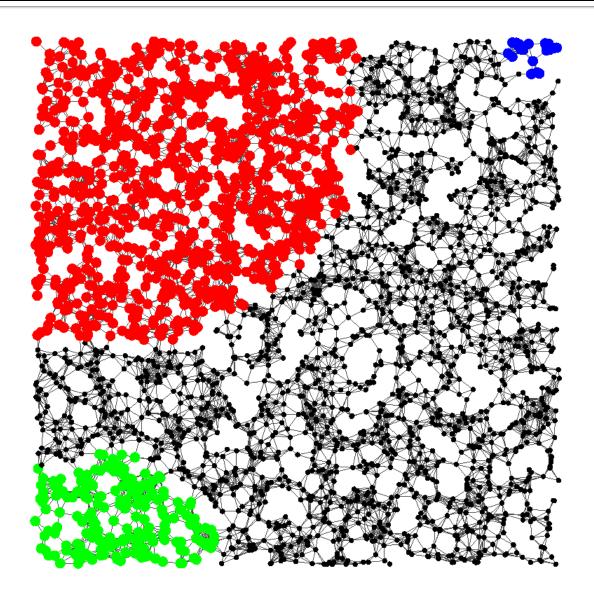
- Approximate PageRank computes PPR in time $\left(\frac{1}{\varepsilon(1-\beta)}\right)$ with residual error $\leq \varepsilon$
 - Power method would take time $O(\frac{\log n}{\varepsilon(1-\beta)})$
- Graph cut approximation guarantee:
 - If there exists a cut of conductance ϕ and volume k then the method finds a cut of conductance $\mathbf{O}(\sqrt{\phi/\log k})$
 - Details in [Andersen, Chung, Lang. Local graph partitioning using PageRank vectors, 2007]

Observations (2)

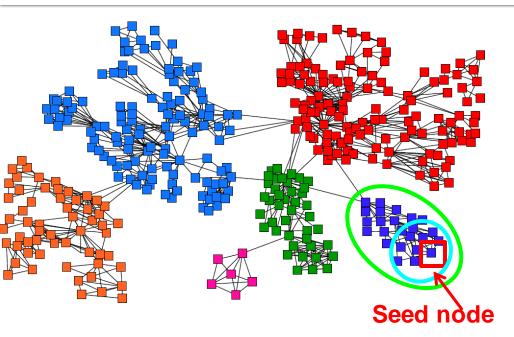
The smaller the ε the farther the random walk will spread and detect far away clusters.

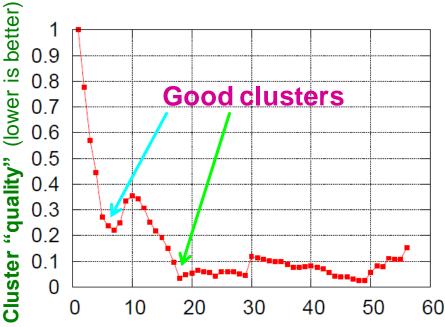


Example



Summary of Approx PPR Alg.





Node rank in decreasing PPR score

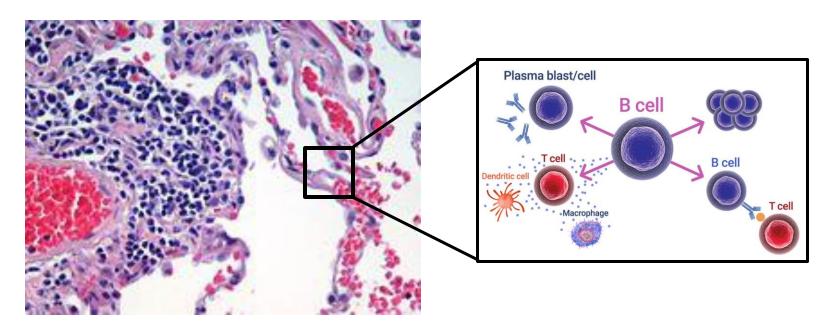
Algorithm summary:

- _
- Pick a seed node s of interest
- Run PPR with teleport set = {s}
- Sort the nodes by the decreasing PPR score
- Sweep over the nodes and find good clusters

Hierarchical Community Detection: Louvain Algorithm

Example: Cells Are Heterogenous

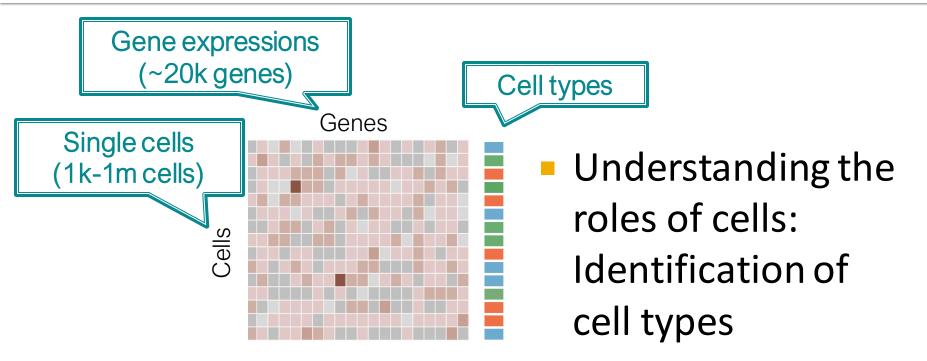
Every cell in a tissue has a specific role



Challenge:

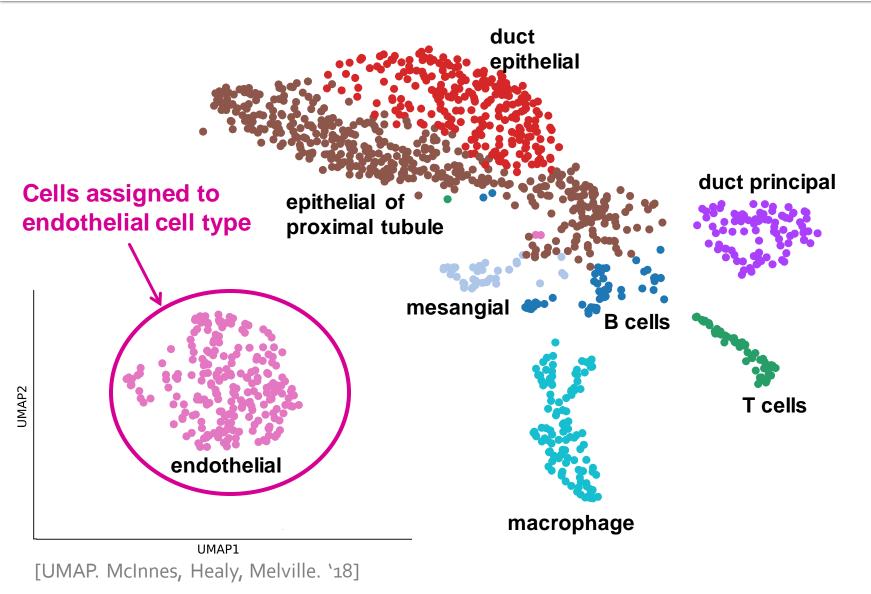
How to determine roles of cells?

Cell Type Identification Task



- Cell type identification task: Given gene expressions of cells, assign cells to cell types
 - Boils down to a clustering task: group cells according to their gene expression similarities

Cell Type Identification Task



Jure Les kovec, Stanford CS246: Mining Massive Datasets

Challenges with Standard Clustering

- Can we use standard clustering methods such as K-means to solve this problem?
- Why standard cluster methods do not work well?
 - Data is very high-dimensional (~20k genes per cell)
 - Data is noisy and sparse (most values will be zero)
 - Number of clusters (cell types) is unknown
 - Cell types are hierarchically organized
 - Definition of cell type is provisional
 - One cell type can have multiple cell subtypes
 - Where to put a threshold on a definition of a cell type?

Idea: Represent Cells as a Graph

 Idea: Construct a graph between data points (cells) and detect hierarchical network communities in a graph

Why is graph a good representation?

- Natural representation: models cell-cell interaction
- Cells with more similar gene expressions are more likely to interact
 - Construct a graph based on similarities between gene expressions of cells
- Hierarchical network communities model well cell type hierarchy

Up Next

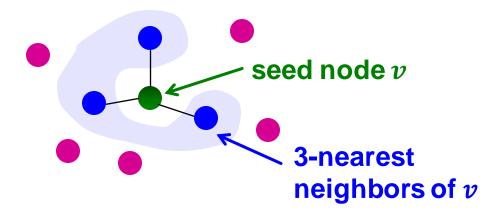
We will cover next:

- 1) How to construct a graph from high-dimensional data?
 - Efficient k-NN graph construction
- 2) How to define network communities?
 - Modularity
- 3) How to detect communities?
 - Louvain algorithm

Efficient K-NN Graph Construction

K-NN Graph

- K nearest neigbor (K-NN) graph: Directed graph with vertex set V and an edge from each v ∈ V to its K most similar objects in V under a given similarity measure
 - E.g., cosine similarity, l_2 distance, l_1 distance



Computing K-NN Graph

Brute force algorithm:

- Takes $O(n^2)$ time
- Only practical for small datasets!

How to efficiently compute K-NN graph?

- NN-Descent [Dong, Charikar, Li. '11]
 - Scalable method for creating approximate K-NN graph
 - Suitable for large-scale datasets
 - lacksquare Empirical cost is around $oldsymbol{O}(oldsymbol{n^{1.14}})$
 - Suitable for distributed implementation (e.g., Map Reduce)

NN-Descent Heuristic

NN-Descent is an iterative refinement algorithm:

- Start with a random KNN graph
 - Each node picks K random other nodes as its nearest neighbors.
- Iteratively refine the list of nearest neighbors of each node:
 - A neighbor of a neighbor could also be my neighbor.
- Keep doing this until convergence.

NN-Descent Algorithm

- Start with a random K-NN list by sampling K items for every node $v \in V$
- Then iteratively for every node $v \in V$:
 - $lackbox{\textbf{B}}[v]$... is the current/approximate K-NN of v
 - $\blacksquare R[v]$... is the current/approximate reverse K-NN of v
 - Reverse K-NN: $R[v] = \{u \in V | v \in B[u]\}$
 - Get general neighbors $B^*[v] = B[v] \cup R[v]$
 - For each general neighbor $u \in B^*[v]$, check the similarity between v and $B^*[u]$ (general neighbors of u are candidates for new neighbors of v)
 - Update nearest neighbors list if similarity is higher compared to the set of current approximate neighbors

Efficient KNN Graph Construction

```
NNDescent(V, \sigma, K):
B[v] = Random \ sample \ of \ K \ items \ V, \ \forall v \in
Loop:
     R = reverse(B)
     B^*[v] = B[v] \cup R[v], \forall v \in V
     c = 0
     for v \in V:
          for u_1 \in B^*[v], u_2 \in B^*[u_1]:
              l = \sigma(v, u_2)
              c = c + updateNN (B[v], \langle u_2, l \rangle)
     return B if c = 0
```

```
m{V} ... datasetm{\partial} m{\sigma} ... similarity oracle m{K} ... number of neighbors m{B}[m{v}] ... approximate neighbors of m{v} m{R}[m{v}] ... approximate reverse neighbors of m{v} m{B}^*[m{v}] ... approximate general neighbors of m{v} m{c} ... counter
```

B[v] is organized as a heap \rightarrow updates cost O(logK)

- reverse(B): $R[v] = \{u \mid \langle v, ... \rangle \in B[u]\}, \ \forall v \in V$ return R
- updateNN(H, (u, l, ...)):
 Update KNN heap H
 return 1 if changed, 0 if not

Example: K=2

Neighbors:

$$B[s] = \{c, d\}$$

Reverse neighbors:

$$R[s] = \{b, c, e\}$$

General neighbors:

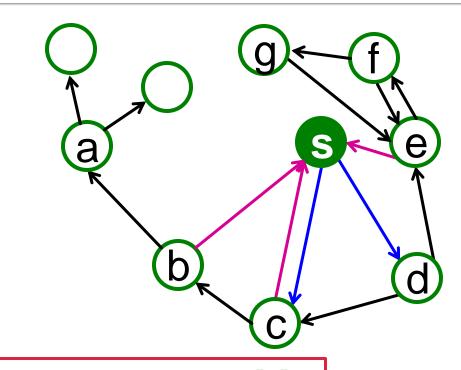
$$\mathbf{B}^*[s] = \{b, c, d, e\}$$

$$\mathbf{B}^*[b] = \{a, c, s\}$$

$$\mathbf{B}^*[c] = \{b, d, s\}$$

$$\mathbf{B}^*[d] = \{c, e, s\}$$

$$\mathbf{B}^*[e] = \{d, f, g, s\}$$



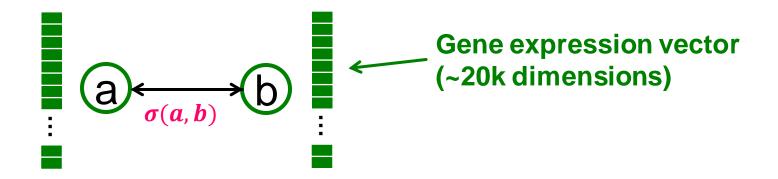
General neighbors of $B^*[s]$ are new candidates for B[s]

We will check $\{a, b, e, f, g\}$ as next candidates for B[s]: Compute $\sigma(s, a)$, $\sigma(s, b)$, $\sigma(s, e)$, $\sigma(s, f)$, $\sigma(s, g)$ and update NNs of s

Arrows denote neighbors of a particular node. For example, arrow from *b* to *s* means that *b* selected *s* as its neighbor (but the opposite does not need to be true).

Cell Type Identification Example

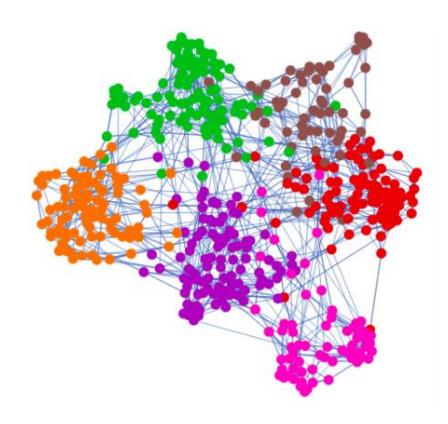
- Which similarity measure σ to use?
 - Cells are compared based on their gene expression profiles
 - Challenge: Number of genes is very high-dimensional



■ Approach: First apply SVD (around 50 dimensions) and then compute l_2 distance in the low-dimensional space

After KNN Graph Construction

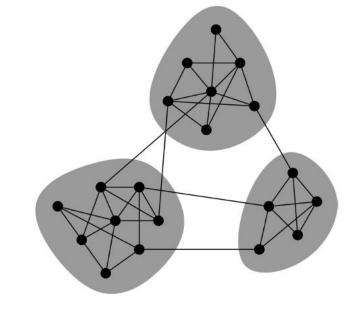
Once we created K-NN graph of cells, how do we define and detect network communities?



Step 2: Defining the metric Modularity Maximization

Network Communities

- Communities: sets of tightly connected nodes
- Define: Modularity Q
 - A measure of how well a network is partitioned into communities
 - Given a partitioning of the network into groups $s \in S$:

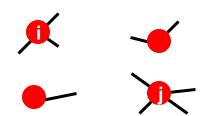


$$Q \propto \sum_{s \in S} [$$
 (# edges within group s) –
(expected # edges within group s)]

Need a null model!

Null Model: Configuration Model

- Given real G on n nodes and m edges,
 construct rewired network G'
 - Same degree distribution but random connections



- Consider G' as a multigraph
- The expected number of edges between nodes i and j of degrees k_i and k_j equals to: $k_i \cdot \frac{k_j}{2m} = \frac{k_i k_j}{2m}$
 - The expected number of edges in (multigraph) G':

$$= \frac{1}{2} \sum_{i \in N} \sum_{j \in N} \frac{k_i k_j}{2m} = \frac{1}{2} \cdot \frac{1}{2m} \sum_{i \in N} k_i \left(\sum_{j \in N} k_j \right) =$$

$$= \frac{1}{4m} 2m \cdot 2m = m$$

Note: $\sum_{u \in V} k_u = 2m$

Modularity

Modularity of partitioning S of graph G:

• Q $\propto \sum_{s \in S} [$ (# edges within group s) – (expected # edges within group s)]

$$Q(G,S) = \underbrace{\frac{1}{2m} \sum_{s \in S} \sum_{i \in s} \sum_{j \in s} \left(A_{ij} - \frac{k_i k_j}{2m} \right) }_{\text{Normalizing const.: -1 < Q < 1}} A_{ij} = 1 \text{ if } i \rightarrow j, 0 \text{ else}$$

Modularity values take range [-1,1]

- It is positive if the number of edges within groups exceeds the expected number
- Q greater than 0.3-0.7 means significant community structure

Community Detection

Idea: We can identify communities by maximizing modularity

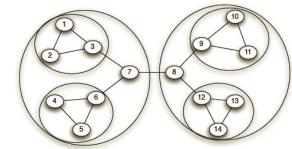
$$Q(G,S) = \frac{1}{2m} \sum_{s \in S} \sum_{i \in s} \sum_{j \in s} \left(A_{ij} - \frac{k_i k_j}{2m} \right)$$

Scalable Step 3: Louvain Algorithm

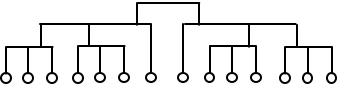
Louvain Algorithm

- Greedy algorithm for community detection
 - $O(n \log n)$ run time
- Supports weighted graphs
- Provides hierarchical communities
- Widely utilized to study large networks because:
 - Fast
 - Rapid convergence
 - High modularity output (i.e., "better communities")

Network and communities:



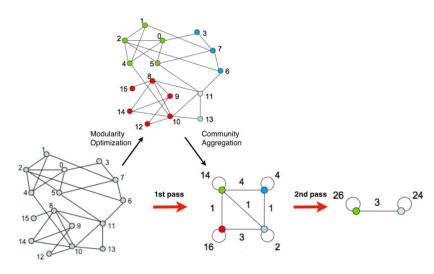
Dendrogram:



Louvain Algorithm: At High Level

- Louvain algorithm greedily maximizes modularity
- Each pass is made of 2 phases:
 - Phase 1: Modularity is optimized by allowing only local changes to node-communities memberships
 - Phase 2: The identified communities are aggregated into super-nodes to build a new network
 - Goto Phase 1

The passes are repeated iteratively until no increase of modularity is possible.



Louvain: 1st phase (Partitioning)

- Put each node in a graph into a distinct community (one node per community)
- For each node i, the algorithm performs two calculations:
 - Compute the modularity delta (ΔQ) when putting node i into the community of some neighbor j
 - Move i to a community of node j that yields the largest gain in ΔQ
- Phase 1 runs until no movement yields a gain

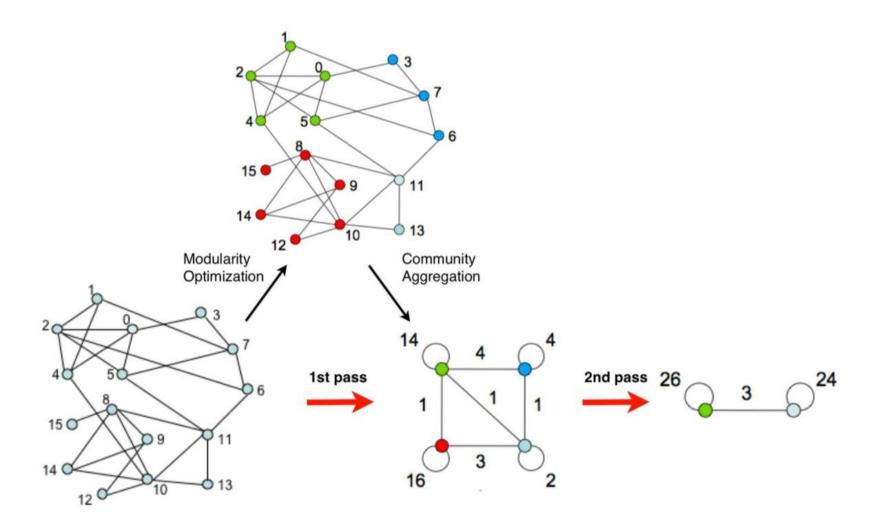
This first phase stops when a local maxima of the modularity is attained, i.e., when no individual node move can improve the modularity.

Note that the output of the algorithm depends on the order in which the nodes are considered. Research indicates that the ordering of the nodes does not have a significant influence on the overall modularity that is obtained.

Louvain: 2nd phase (Restructuring)

- The communities obtained in the first phase are contracted into super-nodes, and the network is created accordingly:
 - Super-nodes are connected if there is at least one edge between the nodes of the corresponding communities
 - The weight of the edge between the two supernodes is the sum of the weights from all edges between their corresponding communities
- Phase 1 is then run on the super-node network

Louvain Algorithm



Back to Detecting Cell Types

Input:

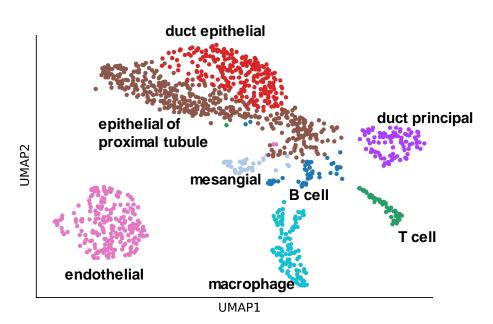
Single-cell gene expression data

Steps:

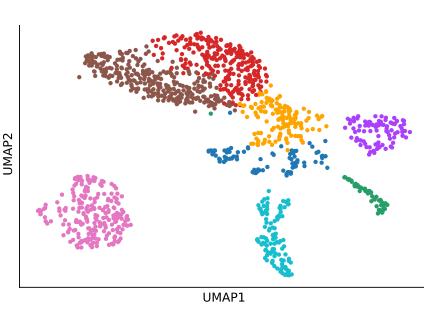
- 1) Apply SVD to cell gene expression data (~50 dim)
- 2) Create K-NN (K=15) graph between the lowdim cell gene expressions
- 2) Apply the Louvain algorithm to identify the clusters

Cell Type Identification Task

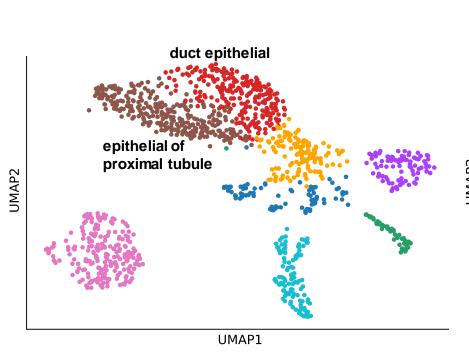
Ground truth annotations

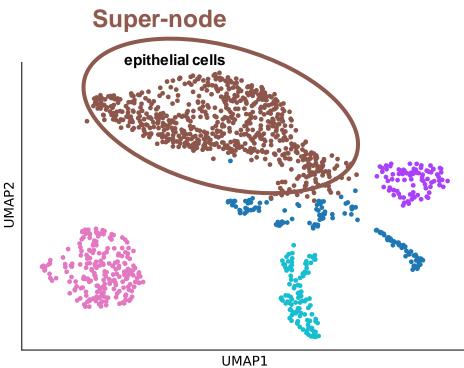


Louvain algorithm



Louvain Hierarchical Groups





Summary: Modularity

Modularity:

- Overall quality of the partitioning of a graph into communities
- Used to determine the number of communities

Louvain modularity maximization:

- Greedy strategy
- Great performance, scales to large networks

Extras: Louvain Algorithm

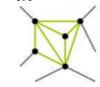
Louvain: Modularity Gain

What is ΔQ if we move node i to community C?

$$\Delta Q(i \to C) = \left[\frac{\sum_{in} + k_{i,in}}{2m} - \left(\frac{\sum_{tot} + k_i}{2m} \right)^2 \right] - \left[\frac{\sum_{in}}{2m} - \left(\frac{\sum_{tot}}{2m} \right)^2 - \left(\frac{k_i}{2m} \right)^2 \right]$$

- where:
 - Σ_{in} ... sum of link weights <u>between</u> nodes in C
 - Σ_{tot} ... sum of <u>all</u> link weights of nodes in C
 - $k_{i,in}$... sum of link weights between node i and C
 - k_i ... sum of <u>all</u> link weights (i.e., degree) of node i







Louvain: Modularity Gain

More in detail:

Modularity contribution **after merging** node *i*

Modularity contribution **before merging** node *i*

$$\Delta Q(i \to C) = \left[\frac{\sum_{in} + k_{i,in}}{2m} - \left(\frac{\sum_{tot} + k_i}{2m} \right)^2 \right] - \left[\frac{\sum_{in}}{2m} - \left(\frac{\sum_{tot}}{2m} \right)^2 - \left(\frac{k_i}{2m} \right)^2 \right]$$

Modularity of i Modularity of C

Self-edge weight

 $k_{i,in}/2$ $\Sigma_{tot} - \Sigma_{in} - (k_{i,in}/2)$ $(k_i - (k_{i.in}/2))$

Edge weight of the resulting supernode from merging C and i

rest of the graph (modeled as a single node) By applying the Modularity definition:

$$Q = rac{1}{2m} \sum_{ij} igg[A_{ij} - rac{k_i k_j}{2m} igg] \delta(c_i, c_j)$$

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- Also need to derive $\Delta Q(D \rightarrow i)$ of taking node i out of community D.
- And then: $\Delta Q = \Delta Q(i \rightarrow C) + \Delta Q(D \rightarrow i)$

Louvain Algorithm

Algorithm 1: Sequential Louvain Algorithm

```
Input: G = (V,E): graph representation.
      Output: C: community sets at each level;
                         Q: modularity at each level.
      Var: \hat{c}: vertex u's best candidate community set.
 1 Loop outer
             C \leftarrow \{\{u\}\}, \forall u \in V ;
             \Sigma_{in}^{c} \leftarrow \sum w_{u,v}, \ e(u,v) \in E, \ u \in c \text{ and } v \in c ;
\Sigma_{tot}^{c} \leftarrow \sum w_{u,v}, \ e(u,v) \in E, \ u \in c \text{ or } v \in c ;
 3
 4
             // Phase 1.
 5
             Loop inner
 6
                     for u \in V and u \in c do
                             // Find the best community for vertex u.
 8
                                                                       \Delta Q_{\underline{u} 	o \underline{c}'}; Modularity gain
                                               argmax
                                      \forall c', \exists e(u,v) \in E, v \in c'
                             if \Delta Q_{u\to\hat{c}} > 0 then
10
                                     // Update \Sigma_{tot} and \Sigma_{in}.
11
                                     \begin{array}{c} \Sigma_{tot}^{\hat{c}} \leftarrow \Sigma_{tot}^{\hat{c}} + w(u) \; ; \; \Sigma_{in}^{\hat{c}} \leftarrow \Sigma_{in}^{\hat{c}} + w_{u \rightarrow \hat{c}} \; ; \\ \Sigma_{tot}^{c} \leftarrow \Sigma_{tot}^{c} - w(u) \; ; \; \Sigma_{in}^{c} \leftarrow \Sigma_{in}^{c} - w_{u \rightarrow c} \; ; \\ \text{// Update the community information.} \end{array}
12
13
14
                                     \hat{c} \leftarrow \hat{c} \cup \{u\} ; c \leftarrow c - \{u\} ;
15
                     if No vertex moves to a new community then
16
                             exit inner Loop;
17
```

Halting criterion for 1st Phase

```
// Calculate community set and modularity.
          Q \leftarrow 0;
19
          for c \in C do
20
               Q \leftarrow Q + \frac{\sum_{in}^{c}}{2m} - (\frac{\sum_{iot}^{c}}{2m})^2;
21
          \underline{C}' \leftarrow \{c\}, \forall c \in C; print \underline{C}' and \underline{Q};
22
         // Phase 2: Rebuild Graph.
23
          V' \leftarrow C'; Communities contracted into super-nodes
24
          E' \leftarrow \{e(c,c')\}, \exists e(u,v) \in E, u \in c, v \in c';
25
          w_{c,c'} \leftarrow \sum w_{u,v}, \forall e(u,v) \in E, u \in c, v \in c'
26
         if No community changes then
27
               exit outer Loop;
28
         V \leftarrow V' : E \leftarrow E' :
29
                                        Halting criterion
                                        for 2<sup>nd</sup> Phase
```

the weights of the edges between the new super-nodes are given by the **sum of the weights of the edges** between vertices in the corresponding two communities