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Oliver Dürr Brown Bag Semiar 16 Apr.

Übersicht



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- Beispiele für Netzwerke
- Was sind Netzwerke
- Überblick Netzwerkanalyse
- Clustering auf Netzwerken
- Graph-Drawing
 - Problemstellung
 - Force-Directed Methoden
 - Optimierung I (Barnes-Hut Approximation)
 - Optimierung II (Multilevel)

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Beispiele für Netzwerke

Social Networks (Zachary Karate Club)







(c) McKenzie's board for manual layout [Nor52]

Terror Networks



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From <u>American Scientist Article</u>



Authorship network

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http://sixdegrees.hu/last.fm/

blame me if an artist is seemingly miscategorised :) Rock is red, metal is dark grey, electronic is orange, hip-hop and rap is blue, jazz is yellow, reggae and ska is magenta, classical music is cyan, country, folk and world music is brown, pop is green. Light grey vertices are unclassified. See the technical details if you are interested in how the categorisation was done.

Protein Protein Interaction Network



444

Biological nets

E.g., Protein-protein interaction (PPI) networks





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a

Definition von Netzwerken

Introduction



What is a network (or graph)?
A set of nodes (vertices) and edges (links)
Edges describe a relationship between the nodes
Some generalizations (see later)
Edges can be (un-)directed, or (un-)weighted





Liste: (undirected graph)

Beschreibungen

Alice	Bob
Alice	Joe
Bob	Joe
Joe	Gilbert

Adjacency matrix

	Alice	Bob	Joe	Gilbert	
Alice		0	1	1	0
Bob		1	0	1	0
Joe		1	1	0	1
Gilbert		0	0	1	0



For undirected and unweighted graphs, adjacency matrix is symmetric and consists of 0's and 1's.

Verallgemeinerungen



Pseudograph / Multigraph



Hypergraph

Eine Kante verbindet mehrere Knoten



Hat self-loops und mehrfache Kanten

Im folgenden nur behandeln wir nur einfache Graphen

© 2010 Genedata AG

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Kurzer Überblick: Netzwerkanalyse

Network Analysis (Overview, biased selection)

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All these networks (social-, actors, genes, …) are similar and can analyzed with the same tools:

Analysis

- General Graph Theory
 - Shortest Path,...
- Graph Drawing
 - Layout Algorithms
- Global Properties
 - Diameter of Graph,
- Centrality Measures
 - E.g. Google's PageRank

Community Detection

- E.g. Friendships
- Modules / Motifs
 - Pattern in the Network
- Comparison
 - How similar are (sub)networks / Chemoinformatik
- Dynamics on Graphs
 - E.g. spreading of rumors / viruses

Properties of typical networks

- Small worldness
 - Six Steps of Seperation
- Scale-freeness
 - There are hubs of abitrary size (Barabasi 1999)

Generation

- From data
 - Correlation with thresholding
 - Graphical Models (e.g Bayesian networks)
- Random
 - Erdös, Barabasi

Software

- Standalone Tools: Cytoscape, Gephi
- R: igraph
- Libraries: Jung, Pajec, Graphviz, prefuse

Surprising properties of networks I

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(Most) "real world" networks have in common that it just takes a few steps to reach any node

(small-worldness) / "6 degrees of separation"

Average path length L~Log(N)





Kevin Bacon at place 507

Power-law distribution L P(k)0.1 0.01 0.001 0.0001 1000 10 100 k $P(k) \sim ck^{-\gamma}$ Google scholar "Emergence of Scaling in Random Networks" Advanced Scholar Search Search Scholar Articles and patents Create email alertResults 1 - 10 of about 6,840. (0.19 se anytime include citations --Emergence of scaling in random networks [PDF] from arxiv.org AL Barabási... - Science, 1999 - sciencemag.org Page 1. DOI: 10.1126/science.286.5439.509, 509 (1999); 286 Science et al. Albert-László Barabási, Emergence of Scaling in Random Networks This copy is for your personal,

Degree Distribution:

Number of edges k

Surprising properties of networks II

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Examples of networks



Graph clustering / Community detection



Task:

Decompose network into parts

Biological relevance:

Given a gene network (PPI, correlation,...) find parts of genes with act together (modules)

Notion: Many ties (edges) within a community, few between communities





NP complete (Brandes 2008)

Community detection

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Heuristic Multiscale Optimization of Modularity



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Multiscale Heuritic of Blondel et al. 2008 <u>http://arxiv.org/abs/0803.0476v2</u>



Heuristic Multiscale Optimization of Modularity



Multiscale Heuristic of Blondel et al. 2008 <u>http://arxiv.org/abs/0803.0476v2</u>



Network of 2'000'000 mobile phone customers. Connected if people had a phone call.

Guess the country...



	Karate	Arxiv	Internet	Web nd.edu	Phone	Web uk-2005 $$	Web WebBase 2001
Nodes/links	34/77	9k/24k	70k/351k	325k/1M	$2.6 \mathrm{M}/6.3 \mathrm{M}$	39M/783M	118M/1B
CNM	.38/0s	.772/3.6s	.692/799s	.927/5034s	-/-	-/-	-/-
PL	.42/0s	.757/3.3s	.729/575s	.895/6666s	-/-	-/-	-/-
WT	.42/0s	.761/0.7s	.667/62s	.898/248s	.56/464s	-/-	-/-
Our algorithm	.42/0s	.813/0s	.781/1s	.935/3s	.769/134s	.979/738s	.984/152mn

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Graph Drawing

Graph Drawing (Definition)



Die Art wie man einen Graph zeichnet ist eine spezielle Darstellung (layout). Beispiel a-f immer der selbe Graph



Masse für die Qualität: Crossing, Längenverteilung der Kanten, Symetrie, ...

Graph has natural layout



zh

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(b) Passes among players during the FIFA World Cup 2010 final. Layout according to (assumed) tactical lineup [PNK10]

Randes in http://cs.brown.edu/~rt/gdhandbook/chapters/social.pdf

Graph has natural layout



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Kinds of Layout (Not Force Directed)



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Circular



Layered (good for DAG)





Force Directed Layout



Forces:

- Vertex-Vertex Repulsion: Electrically charged particles (nodes)
- Edges: Attraction: Springs that connect particles via edges;
- (Viscosity to damp movements)

See also:

http://vimeo.com/4356593 http://vimeo.com/3206267

3 historical models

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Eades Spring embedder (1984)

Springs and artificial repulsion forces (logarithmic)

Fruchterman-Reingold (1991) Forces artificial springs and repulsion Optimization: Steepest decent, step size ~ to temperatur

Kamanda and Kawai (1989) Only Springs but with rest length

Details of the Intercation (Springs)

Spring Forces:

Hook's law ||x(from(ei)) - x(to(ei))|| used in prefuse library

FR found that they had more success using a quadratic spring force ||x(from(ei)) - x(to(ei))||^2 better for local minima backed by Jiggle [Jiggle DISS]

Eades log(||x(from(ei)) - x(to(ei))|| / x0),

Logarithmic spring force leads to an unaesthetically high degree of variance in the edge lengths [Joggle DISS]

Kamada and Kawai (only Springs)

Rest length of the corresponding spring is proportional to **shortestPath(vi, vj) Force (1 / shortestPath(vi, vj)) • | ||xi - xj|| - c • shortestPath(vi, vj) |** Problem n^2 Springs

Details of the interactions (V-V Forces)

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Vertex-Vertex Forces

Kamanda Kawai

(no such force) just springs with rest length

Eades, prefuse-library

1/||xi - xj||^2

Fruchterman Reingold

1/||xi - xj||

Side remark (Column interaction in 2d log(||xi - xj|| → Force 1/r as in FR)

Detail: Forces

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Additional Term in source Fruchterman-Reingold in R Expected Observe Observe Expected Observe Observe Observe File: laugut.c. method igraph. layout fruchterman. reingold An additional undocumented

yd=MATRIX(*res, j, 1)-MATRIX(*res, k, 1); zd=MATRIX(*res, j, 2)-MATRIX(*res, k, 2); ded=sqrt(xd*xd+yd*yd+zd*zd); /*Get dyadic euclidean distance* if (ded != 0) { /*Rescale differences to length 1*/ xd/=ded; yd/=ded; zd/=ded; /*Calculate repulsive "force"*/ rf=frk*frk*(1.0/ded-ded*ded/repulserad); } else { /* ded is exactly zero. Use some small random displacement. */ xd=RNG_NORMAL(0,0.1); yd=RNG_NORMAL(0,0.1); zd=RNG_NORMAL(0,0.1); rf=RNG_NORMAL(0,0.1); 3 MATRIX(dxdydz, j, 0)+=xd*rf; /*Add to the position change vector*/ MATRIX(dxdydz, k, 0)-=xd*rf; MATRIX(dxdydz, j, 1)+=yd*rf;

An additional undocumented V-V force with r²

Keeps disconnected graphs together. Switched of by setting parameter repluserad high.

Demo Force Directed

Demo dynamic of layout

g <- graph.ring(100, directed=FALSE)

wt <- multilevel.community(g)</pre>

V(g)\$color <- wt\$membership

I <- layout.random(g)</pre>

for (i in 1:100) {

I <- layout.fruchterman.reingold(g, params=list(niter=5, start=I, repulserad=1e30))

#l <- layout.fruchterman.reingold(g, params=list(niter=4000, start=l))</pre>

plot(g,layout=l,vertex.size=3, vertex.label=NA, main=paste0("FR ", i))

Sys.sleep(1);

}

I <- layout.fruchterman.reingold(g, params=list(niter=5000, start=l, repulserad=1e30))
plot(g,layout=l,vertex.size=3, vertex.label=NA, main=paste0("FR ", i))</pre>

Running Times

Number of Edges: **n**

```
Time per Iteration θ(n^2)
```

Number of Iterations until convergence (poorly understood) but generally assumed to be ~ n

Eades / Fruchterman Reingold θ(n^3)

Kamanda Kawei Different naïve θ(n^3) Spezialized approach θ(nm log n)

Pros and Cons force directed

Pros (from wikipedia)

- Good-quality results
 - At least for graphs of medium size (up to 50–100 vertices)... following criteria: uniform edge length, uniform vertex distribution, symmetry.
- Flexibility
 - Force-directed algorithms can be easily adapted and extended to fulfill additional aesthetic criteria.
- Simplicity
 - Typical force-directed algorithms are simple and can be implemented in a few lines of code. Other classes of graph-drawing algorithms, like the ones for orthogonal layouts, are usually much more involved.
- Interactivity
 -This makes them a preferred choice for dynamic and online graph-drawing systems.
- Strong theoretical foundations
 - ...statisticians have been solving similar problems in multidimensional scaling (MDS) since the 1930s, and physicists also have a long history of working with related n-body problems –

Ways to do Graph Drawing (Force Directed)

Cons (from wikipedia)

- High running time
 - The typical force-directed algorithms are in general considered to have a running time equivalent to O(n3), where n is the number of nodes of the input graph. This is because the number of iterations is estimated to be O(n), and in every iteration, all pairs of nodes need to be visited and their mutual repulsive forces computed O(n2). Solution: Barnes-Hut Approximation.
- Poor local minima
 - ... The problem of poor local minima becomes more important as the number of vertices of the graph increases. For example, using the Kamada–Kawai algorithm[10] to quickly generate a reasonable initial layout and then the Fruchterman–Reingold algorithm[11] to improve the placement of neighbouring nodes. Another technique to achieve a global minimum is to use a **multilevel approach**.

Lets tackle the cons...

How to draw it faster I (Barnes-Hut)

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two galaxies colliding (Nice Movie)

Particels which are far enough away can be approximated by the center of mass. Stored on the nodes in the search tree Has been used for simulating e.g. many particel problems.

In space The search Tree (quadtree) NW NO NO NW SW SO SO NW SO / NO NO SO NW NW NW SW NO NO SO SW NO SW NW SO SO SO SW SW

How to draw it faster I (Barnes-Hut)

Barnes-Hut Approximation (from: $O(n^2)$ to $O(n \log n)$)

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Barnes Hut vs. no approximation

No BH 30 sec

BH 0.8 5.5 sec

Similar layout in 1/6 of the time.

Scaling n log(n) vs. n²

How to draw it faster II (Multilevel)

Problem: unfolding takes quite some time

Simple Force Directed http://www.youtube.com/watch?v=-K5zTCrQ_wc&feature=plcp

• Input: G⁰ = (V;E) with random initial placements

Multilevel: Coarsen G⁰ → (G⁰,G¹,G²...G^{k·1},G^k) For i=k to i=0, Compute the layout of Gⁱ /* On GPU */ Interpolate the initial positions of G^{i·1}

Output: G⁰ = (V'; E) with final placements

Different ways to coarsen:

See e.g. An Experimental Evaluation of Multilevel Layout Methods Bartel et al 2012

Why not take to coarsen?

ML layout algorithm at work

Multilevel Layout http://www.youtube.com/watch?v=J_wkNESO65k&feature=plcp

