# **Models of Science**

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# Four Parts:

- 1. Conceptualizing Science
- 2. Model Inspirations from Other Sciences
- 3. Models of Science
- 4. Tools to Model and Map Science

















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# Modeling of Science Learning from Epidemiology



### Modeling Science Learning from Economics



Self amplifying downward spiral | 'systemic' meltdown with intertwined breakdowns | 'war room' analyses | market wind tunnel |power market test bed | Regulators feel duty-bound to adhere to generally accepted and well-vetted techniques

"... while any new technical device or medical drug has extensive testing for efficiency, reliability and safety before it ever hits the market, we still implement new economic measures without any prior testing." Dirk Helbing

# Modeling Science Learning from Economics



Logicland Participative Global Simulation - Michael Ashauer, Maia Gusberti, Nik Thoenen - 2002

# Mapping Science Learning from Meteorology



Named Storms, available online at http://svs.gsfc.nasa.gov/vis/a000000/a003200/a003279

## Patch-working Models/Studies/Maps of Science Learning from Astronomy



home | project summary | people | gallery | news | related links | bibliography | data | use

#### Gallery of Solved Images

In the images below, the red circles are stars our algorithm automatically detects in the image, and the green circles are stars from our master index which appear in the query image. Nebulae, constellations and other objects can be automatically overlayed on the image after it has been solved.

A shot of the Great Nebula, by Jerry Lodriguss (c.2006), from astropix.com



<u>http://www.astrometry.net/gallery.html</u> <u>http://cosmo.nyu.edu/hogg/research/2006/09/28/astrometry\_google.pdf</u>

#### Patch-working Models/Studies/Maps of Science Learning from Seismology



Tectonic Movements and Earthquake Hazard Predictions - Martin W. Hamburger, Lou Estey, Chuck Meertens, Elisha Hardy - 2005

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#### An introduction to modeling science: Basic model types, key definitions, and a general framework for the comparison of process models

Katy Börner, Kevin W. Boyack, Staša Milojević, Steven Morris. (2011) In Scharnhorst, Andrea, Börner, van den Besselaar (Eds) Models of Science Dynamics. Springer Verlag.

#### **Modeling Process**

- 1. Formulation of a scientific hypothesis about the identification of a specific structure or dynamics. Often, this hypothesis is based on analysis of patterns found in empirical data.
- 2. Algorithm design and implementation using either tools (e.g., NetLogo, RePast) or custom codes that attempt to mathematically describe the structure or dynamics of interest.
- 3. Simulated data are calculated by running the algorithm and validated by comparison with empirical data.
- 4. Resulting insights frequently inspire new scientific hypotheses, and the model is iteratively refined or new models are developed.



# An introduction to modeling science: Basic model types, key definitions, and a general framework for the comparison of process models

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# Descriptive Models vs. Process Models

# **Descriptive Models**

Aim to describe the major features of a (typically static) data set, e.g., statistical patterns of article citation counts, networks of citations, individual differences in citation practice, the composition of knowledge domains, and the identification of research fronts as indicated by new but highly cited papers.

### Bibliometrics, Scientometrics, or KDVis

### **Process Models**

Aim to simulate, statistically describe, or formally reproduce the statistical and dynamic characteristics of interest. Of particular interest are models that "conform to the measured data not only on the level where the discovery was originally made but also at the level where the more elementary mechanisms are observable and verifiable" (Willinger, Govindan, Jamin, Paxson, & Shenker, 2002), p.2575.

Statistical Physics and Sociology



# **Descriptive Models**

# **Examples:**

- Detect advances of scientific knowledge via "longitudinal mapping" (Garfield, 1994).
- > Synthesis of specialty narratives from co-citation clusters (Small, 1986).
- Identify cross-disciplinary fertilization via "passages through science" (Small, 1999, 2000).
- > Understand scholarly information foraging (Sandstrom, 2001).
- Knowledge discovery in un-connected terms (Swanson & Smalheiser, 1997).
- Determine areas of expertise for specific researcher, research group via "invisible colleges" (note that researchers self definition might differ from how field defines him/her) (Crane, 1972).
- Identify profiles of authors, also called CAMEOS, to be used to for document retrieval or to map an author's subject matter and studying his/her publishing career, or to map the social and intellectual networks evident in citations to and from authors and in co-authorships (White, 2001).



- > Identification of scientific frontiers <u>http://www.science-frontiers.com/</u>.
- > ISI's Essential Science Indicators <u>http://essentialscience.com/</u>
- Import-export studies (Stigler, 1994).
- Evaluation of 'big science' facilities using 'converging partial indicators' (Martin, 1996; Martin & Irvine, 1983).
- Input (levels of funding, expertise of scientists, facilities used) output (publications, patents, Nobel prices, improved health, reduced environment insults, etc. - influenced by political, economic, financial, and legal factors studies (Kostroff & DelRio, 2001).
- > Determine influence of funding on research output (Boyack & Borner, 2002).
- > How to write highly influential paper (van Dalen & Henkens, 2001).



# **Process Models**

Can be used to predict the effects of

- Large collaborations vs. single author research on information diffusion.
- Different publishing mechanisms, e.g., E-journals vs. books on co-authorship, speed of publication, etc.
- Supporting interdisciplinary collaborations (shallow science? or decrease in duplication?).
- Many small vs. one large grant on # publications, Ph.D. students, etc.
- Resource distribution on research output.
- ▶ ...

In general, process model provide a means to analyze the structure and dynamics of science -- to study science using the scientific methods of science as suggested by Derek J. deSolla Price about 40 years ago.

# We now do have the data, code and compute power to do this!

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**Process Models** 

In *Sociology*, several mathematical models of network evolution have been developed (Banks & Carley, 95). Most assume a <u>fixed number of edges</u>.

Snijders' Simulation Investigation for Empirical Network Analysis (SIENA) (<u>http://stat.gamma.rug.nl/snijders/siena.html</u>) is a probabilistic model for the evolution of social networks. It assumes a <u>directed graph with a fixed set of actors</u>.

Recent work in *Statistical Physics* aims to design models and analytical tools to analyze the statistical mechanics of topology and dynamics of real world networks. Of particular interest is the identification of elementary mechanisms that lead to the emergence of *small-world* (Albert & Barabási, 2002; Watts, 1999) and *scale free network structures* (Barabási, Albert, & Jeong, 2000). The models assume nodes of <u>one type</u> (e.g., web page, paper, author).

Examples:

- **Watts-Strogatz Model** for Small World Networks
- > Albert-Barabasi Model for Scale Free Networks



## The Watts-Strogatz Model for Small World Networks

First model that generates graphs with small average path length and high clustering coefficients.

- Starting configuration is a regular lattice.  $\geq$
- Each edge is examined and is redirected with a probability p to another target node (chosen randomly).

Regular network (left) drastically changes from a set of tiny isolated clusters of nodes to a giant cluster joined by almost everybody.



tice (left) a

(Source: D.J. Watts and S. Strogatz. Collective Dynamics of Small-World' Networks. Nature, Vol. 393(6):pp. 440-442, June 1998.)



Figure 2. As the probability of rewiring increases in the Watts-Strogatz model, the characteristic path length falls off long before the clustering coefficient drops. Results are from 2,000 random graphs, each with 300 vertices and 900 edges.

C(p) and l(p) as a function of rewiring probability p.



random

effects

lattice-like (several neighbors) regular + random





#### The Barabasi-Albert (BA) Model for Scale Free Networks

Many large networks are scale free, their degree distribution follows a power law for large k. Random graph theory and the small world model cannot reproduce this feature.

- (1) Growth: Starting with a small number  $(m_0)$  of nodes, at every time step, we add a new node with  $m(\le m_0)$  edges that link the new node to m nodes already present in the system.
- (2) Preferential attachment: The probability p that a new node will be connected to node i depends on the degree k<sub>i</sub> of node i, such that

$$\mathbf{p}(k_i) = \frac{k_i}{\sum_j k_j}.$$

After t time-steps the network has  $N = t+m_0$  nodes and mt edges.

This network evolves into a stationary scale-free state with the probability that a node has k edges following a power law with an exponent  $\gamma_{BA} = 3$ .

(Source: A.-L. Barabasi, R. Albert, Emergence of scaling in random networks, Science 286 (1999) 509512.)



FIG. 23. A simple deterministic growing graph. At time  $t\,=\,0,$  the graph is a triangle. At each time step every edge of the graph generates a new vertex which connects to both ends of the edge.



growing network [166]. In the initial configuration, t = 2, three vertices are present, s = 0, 1, 2 (a). At each increment of time, a new vertex with two edges is added. These edges are attached to the ends of a randomly chosen edge of the network.

# Information Diffusion Among Major U.S. Research Institutions

Börner, Katy, Penumarthy, Shashikant, Meiss, Mark & Ke, Weimao. (2006). Mapping the Diffusion of Information among Major U.S. Research Institutions. Scientometrics. Vol. 68(3), 415 - 426.

#### **Questions:**

- 1. Does space still matter in the Internet age, i.e., does one still have to study and work at major research institutions in order to have access to high quality data and expertise and to produce high quality research?
- 2. Does the Internet lead to more global citation patterns, i.e., more citation links between papers produced at geographically distant research instructions?

#### **Contributions:**

- Answer to Q1 is YES.
- Answer to Q2 is NO.
- Novel approach to analyzing the dual role of institutions as information producers and consumers and to study and visualize the diffusion of information among them.



### 20-Year PNAS Dataset (1982-2001)

Coverage in terms of time span, total number of papers, and complete author's work



#### **Citation Matrix**

Unsymmetrical direct citation linkage patterns among the top 500 institutions. High peak values in the diagonal reflect the high amount of self-citations for all institutions. Medium peak horizontal and vertical lines denote references from and citations to papers written at Harvard University.



#### Information Sources (Export) and Sinks (Import)

Calculate ratio of the number of citations received by an institution divided by the sum of received citations and references made, multiplied by 100.

131 have a value between 0-40% acting mostly as information producers = information sources.

71 have a value between 60-100% and act mostly as information consumers – they reference a large number of papers but the number of citations they receive is comparably low = information sinks. (*Tobler*, 1995)

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#### **Geographic Location of Received Citations**

Unsymmetrical direct citation linkage patterns among the top 500 institutions. High peak values in the diagonal reflect the high amount of self-citations for all institutions. Medium peak horizontal and vertical lines denote references from and citations to papers written at Harvard University.



#### Information Flow Among the Top-5 Consumers and Their Top-10 Producers



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#### **Changes in Citation Behavior Over Time**

Unsymmetrical direct citation linkage patterns among the top 500 institutions. High peak values in the diagonal reflect the high amount of self-citations for all institutions. Medium peak horizontal and vertical lines denote references from and citations to papers written at Harvard University.



#### Modeling the Co-Evolving Author-Paper Networks

Börner, Katy, Maru, Jeegar & Goldstone, Robert. (2004). The Simultaneous Evolution of Author and Paper Networks. PNAS. Vol. 101 (Suppl. 1), 5266-5273.



#### The TARL Model (Topics, Aging, and Recursive Linking) incorporates

- A partitioning of authors and papers into topics,
- > Aging, i.e., a bias for authors to cite recent papers, and
- A tendency for authors to cite papers cited by papers that they have read resulting in a rich get richer effect.

The model attempts to capture the roles of authors and papers in the production, storage, and dissemination of knowledge.

#### **Model Assumptions**

- > Co-author and paper-citation networks co-evolve.
- Authors come and go.
- Papers are forever.
- > Only authors that are 'alive' are able to co-author.
- > All existing (but no future) papers can be cited.
- Information diffusion occurs directly via co-authorships and indirectly via the consumption of other authors' papers.
- Preferential attachment is modeled as an *emergent property* of the elementary, local networking activity of authors reading and citing papers, but also the references listed in papers.



#### Aging function





Year	#p	#a	#r	iic	allca
1981	1624	3953	0	756	8,2
1982	1040	5200	31200	112161	
1983	1118	5590	33540	21397	1 8
1984	1197	5985	35910	10224	1 8
1985	1275	6375	38250	6184	
1986	1353	6765	40590	4687	
1987	1432	7160	42960	3573	
1988	1510	7550	45300	2816	
1989	1589	7945	47670	2219	
1990	1667	8335	50010	1853	
1991	1745	8725	52350	1634	
1992	1824	9120	54720	1431	1 8
1993	1902	9510	57060	1167	: 3
1994	1981	9905	59430	1040	
1995	2059	10295	61770	767	
1996	2137	10685	64110	632	
1997	2216	11080	66480	522	
1998	2294	11470	68820	400	1
1999	2373	11865	71190	265	
2000	2451	12255	73530	125	
2001	2529	12645	75870	0	
Total	37316		1070760	173853	

#### Model Validation

The properties of the networks generated by this model are validated against a 20-year data set (1982-2001) of documents of type article published in the Proceedings of the National Academy of Science (PNAS) – about 106,000 unique authors, 472,000 coauthor links, 45,120 papers cited within the set, and 114,000 citation references within the set.







the power law exponent as authors are now restricted to cite papers in their own topics area.

Aging: With increasing b, and hence increasing the number of older papers cited as references, the clustering coefficient decreases. Papers are not only clustered by topic, but also in time, and as a community becomes increasingly nearsighted in terms of their citation practices, the degree of temporal clustering increases.

#### **References/Recursive**

Linking: The length of the chain of paper citation links that is followed to select references for a new paper also influences the clustering coefficient. Temporal clustering is ameliorated by the practice of citing (and hopefully reading!) the papers that were the earlier inspirations for read papers.

# Topics

Aging Function

Model Initialization Values

# Authors in Start Year

# Papers in Start Year

# Co-Author(s) per Author

# Papers Consumed (Referenced) per Pape

# Papers Produced per Author each Year

# Levels References are Considered

0

1

5

1

1

2 # Years



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Börner, Katy. (March 2011). Plug-and-Play Macroscopes. *Communications of the ACM*, 54(3), 60-69.

Video and paper are at <u>http://www.scivee.tv/node/27704</u>



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# Type of Analysis vs. Level of Analysis

	Micro/Individual	Meso/Local	Macro/Global
	(1-100 records)	(101–10,000 records)	(10,000 < records)
Statistical Analysis/Profiling	Individual person and their expertise profiles	Larger labs, centers, universities, research domains, or states	All of NSF, all of USA, all of science.
Temporal Analysis	Funding portfolio of one individual	Mapping topic bursts	113 Years of Physics
(When)		in 20-years of PNAS	Research
Geospatial Analysis (Where)	Career trajectory of one individual	Mapping a states intellectual landscape	PNAS Publications
Topical Analysis	Base knowledge from which one grant draws.	Knowledge flows in	VxOrd/Topic maps of
(What)		Chemistry research	NIH funding
Network Analysis (With Whom?)	NSF Co-PI network of one individual	Co-author network	NSF's core competency



#### Sci<sup>2</sup> Tool: Algorithms

#### Preprocessing

Extract Top N% Records Extract Top N Records Normalize Text Slice Table by Line

Extract Top Nodes Extract Nodes Above or Below Value Delete Isolates

Extract top Edges Extract Edges Above or Below Value Remove Self Loops Trim by Degree MST-Pathfinder Network Scaling Fast Pathfinder Network Scaling

Snowball Sampling (in nodes) Node Sampling Edge Sampling

Symmetrize Dichotomize

Multipartite Joining

Geocoder

Extract ZIP Code

#### Modeling

Random Graph Watts-Strogatz Small World Barabási-Albert Scale-Free TARL

Analysis Network Analysis Toolkit (NAT) Unweighted & Undirected Node Degree Degree Distribution

> K-Nearest Neighbor (Java) Watts-Strogatz Clustering Coefficient Watts Strogatz Clustering Coefficient over K

Diameter Average Shortest Path Shortest Path Distribution Node Betweenness Centrality

Weak Component Clustering Global Connected Components

Extract K-Core Annotate K-Coreness

HITS

Weighted & Undirected

Clustering Coefficient Nearest Neighbor Degree Strength vs Degree Degree & Strength Average Weight vs End-point Degree Strength Distribution Weight Distribution Randomize Weights

Blondel Community Detection

HITS Unweighted & Directed Node Indegree Node Outdegree Indegree Distribution Outdegree Distribution

> K-Nearest Neighbor Single Node in-Out Degree Correlations

Dyad Reciprocity Arc Reciprocity Adjacency Transitivity

Weak Component Clustering Strong Component Clustering

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Extract K-Core Annotate K-Coreness

#### HITS PageRank Weighted & Directed HITS

Weighted PageRank

#### Textual Burst Detection

Sci<sup>2</sup> Tool: Algorithms cont.

#### Visualization

GnuPlot GUESS Image Viewer

Radial Tree/Graph (prefuse alpha) Radial Tree/Graph with Annotation (prefuse beta) Tree View (prefuse beta) Tree Map (prefuse beta) Force Directed with Annotation (prefuse beta) Fruchterman-Reingold with Annotation (prefuse beta)

DrL (VxOrd) Specified (prefuse beta)

Horizontal Bar Graph Circular Hierarchy Geo Map (Circle Annotation Style) Geo Map (Colored-Region Annotation Style) Science Map (Circle Annotation)

#### Scientometrics

Remove ISI Duplicate Records Remove Rows with Multitudinous Fields Detect Duplicate Nodes Update Network by Merging Nodes

Extract Directed Network Extract Paper Citation Network Extract Author Paper Network

#### Extract Co-Occurrence Network

Extract Word Co-Occurrence Network Extract Co-Author Network Extract Reference Co-Occurrence (Bibliographic Coupling) Network

Extract Document Co-Citation Network

# **Soon:** Database support for ISI and NSF data.



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Statistical Analysis/Profiling   Individual person and their expertise profiles   Larger labs, centers, universities, research lomains or states   All of N: I o	Statistical Analysis/Profiling   Individual person and their expertise profiles   Larger labs, centers, universities, research domains or states   All of Nt all of sci (when)     Temporal Analysis (When)   Funding portfolio of one individual   ic bursts f PNAS   I13 Years of P Research     Geospatial Analysis (Where)   Career trajectory of on individual   Intellectual I   PNAS     Topical Analysis (What)   Career trajectory of on individual   Intellectual I   VxOrd/Topic I     Network Analysis (With Whom?)   NSI one   Vord for the search   NIH's	Statistical Analysis/Profiling   Individual person and their expertise profiles   Larger labs, centers, universities, research formation, or states   All of N all of Sci all of Sci al		Micro/Individual (1-100 records)	Meso/Local (101–10,000 records)	Macro/Global (10,000 < records)
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Shiffrin, Richard M. and Börner, Katy (Eds.) (2004). **Mapping Knowledge Domains**. Proceedings of the National Academy of Sciences of the United States of America, 101(Suppl\_1). http://www.pnas.org/content/vol101/suppl\_1/

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All papers, maps, tools, talks, press are linked from http://cns.iu.edu

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