Setting the Stage: Modelling and Visualizing Science and Technology Developments

Katy Börner, William Rouse, H. Eugene Stanley, and Paul Trufio

NAS Sackler Colloquium on Modeling and Visualizing Science and Technology Developments
Arnold and Mabel Beckman Center, Irvine, California

December 4, 2017

14 years ago:

The Arthur M. Sackler Colloquium on **Mapping Knowledge Domains** was held at the Arnold and Mabel Beckman Center of the National Academies of Sciences and Engineering in Irvine, CA, May 9–11, 2003.

It showcased ongoing developments in this research area and provided pointers toward future developments.

136 pages

[https://doi.org/10.17226/11048](https://doi.org/10.17226/11048)
Widely Used Models

Weather Forecast
Oil Depletion
Seismic Hazards
Epidemic Models
Chess Playing and Other Gaming Models
<table>
<thead>
<tr>
<th>DAY</th>
<th>DESCRIPTION</th>
<th>HIGH / LOW</th>
<th>PRECIP</th>
<th>WIND</th>
<th>HUMIDITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>TODAY</td>
<td>Sunny</td>
<td>82°/55°</td>
<td>☀️ 0%</td>
<td>S 6 mph</td>
<td>53%</td>
</tr>
<tr>
<td>SUN</td>
<td>Sunny</td>
<td>77°/58°</td>
<td>☀️ 0%</td>
<td>WSW 6 mph</td>
<td>62%</td>
</tr>
<tr>
<td>MON</td>
<td>Partly Cloudy</td>
<td>67°/49°</td>
<td>☁️ 20%</td>
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</tr>
<tr>
<td>TUE</td>
<td>Partly Cloudy</td>
<td>76°/51°</td>
<td>☁️ 0%</td>
<td>S 6 mph</td>
<td>32%</td>
</tr>
<tr>
<td>WED</td>
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<td>73°/53°</td>
<td>☁️ 0%</td>
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<td>47%</td>
</tr>
<tr>
<td>THU</td>
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<td>73°/53°</td>
<td>☁️ 0%</td>
<td>SSE 6 mph</td>
<td>53%</td>
</tr>
<tr>
<td>FRI</td>
<td>Partly Cloudy</td>
<td>71°/53°</td>
<td>☁️ 10%</td>
<td>SSE 6 mph</td>
<td>63%</td>
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<tr>
<td>SAT</td>
<td>Showers</td>
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<td>76%</td>
</tr>
<tr>
<td>SUN</td>
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<td>☁️ 20%</td>
<td>SSE 5 mph</td>
<td>61%</td>
</tr>
<tr>
<td>MON</td>
<td>Showers</td>
<td>68°/50°</td>
<td>⛈️ 40%</td>
<td>SE 8 mph</td>
<td>62%</td>
</tr>
<tr>
<td>TUE</td>
<td>Partly Cloudy</td>
<td>66°/48°</td>
<td>⛈️ 20%</td>
<td>SE 5 mph</td>
<td>62%</td>
</tr>
<tr>
<td>WED</td>
<td>Partly Cloudy</td>
<td>68°/50°</td>
<td>⛈️ 20%</td>
<td>ESE 7 mph</td>
<td>62%</td>
</tr>
<tr>
<td>THU</td>
<td>Mostly Sunny</td>
<td>69°/51°</td>
<td>⛈️ 10%</td>
<td>ENE 7 mph</td>
<td>57%</td>
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<tr>
<td>FRI</td>
<td>Partly Cloudy</td>
<td>70°/52°</td>
<td>⛈️ 0%</td>
<td>ESE 7 mph</td>
<td>54%</td>
</tr>
</tbody>
</table>

# Irvine, CA 10 Day Weather

**Retrieved on 12/03/2017, 9:28am**

<table>
<thead>
<tr>
<th>DAY</th>
<th>DESCRIPTION</th>
<th>HIGH / LOW</th>
<th>PRECIP</th>
<th>WIND</th>
<th>HUMIDITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>TODAY</td>
<td>Partly Cloudy</td>
<td>69°/51°</td>
<td>10%</td>
<td>SSW 7 mph</td>
<td>76%</td>
</tr>
<tr>
<td>MON</td>
<td>Partly Cloudy</td>
<td>73°/52°</td>
<td>0%</td>
<td>ENE 18 mph</td>
<td>18%</td>
</tr>
<tr>
<td>TUE</td>
<td>Partly Cloudy/Wind</td>
<td>74°/49°</td>
<td>0%</td>
<td>NE 23 mph</td>
<td>11%</td>
</tr>
<tr>
<td>WED</td>
<td>Sunny</td>
<td>77°/53°</td>
<td>0%</td>
<td>NNE 7 mph</td>
<td>16%</td>
</tr>
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<td>THU</td>
<td>Partly Cloudy</td>
<td>79°/53°</td>
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<td>NE 9 mph</td>
<td>16%</td>
</tr>
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<td>FRI</td>
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<td>19%</td>
</tr>
<tr>
<td>SAT</td>
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<td>78°/53°</td>
<td>0%</td>
<td>E 5 mph</td>
<td>24%</td>
</tr>
<tr>
<td>SUN</td>
<td>Partly Cloudy</td>
<td>76°/53°</td>
<td>0%</td>
<td>S 4 mph</td>
<td>27%</td>
</tr>
<tr>
<td>MON</td>
<td>Sunny</td>
<td>74°/53°</td>
<td>0%</td>
<td>SSW 5 mph</td>
<td>27%</td>
</tr>
<tr>
<td>TUE</td>
<td>Mostly Sunny</td>
<td>75°/54°</td>
<td>0%</td>
<td>SSW 5 mph</td>
<td>35%</td>
</tr>
<tr>
<td>WED</td>
<td>Mostly Sunny</td>
<td>76°/54°</td>
<td>0%</td>
<td>SSE 5 mph</td>
<td>38%</td>
</tr>
<tr>
<td>THU</td>
<td>Sunny</td>
<td>76°/54°</td>
<td>0%</td>
<td>SSW 6 mph</td>
<td>40%</td>
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### Irvine, CA 10 Day Weather

#### Retrieved on 11/25/2017, 9:27am

<table>
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<th>DESCRIPTION</th>
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<th>PRECIP</th>
<th>WIND</th>
<th>HUMIDITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>SUN DEC 3</td>
<td>Partly Cloudy</td>
<td>69°'/50°'</td>
<td>20%</td>
<td>SSE 5 mph</td>
<td>61%</td>
</tr>
<tr>
<td>MON DEC 4</td>
<td>Showers</td>
<td>68°'/50°'</td>
<td>40%</td>
<td>SE 8 mph</td>
<td>62%</td>
</tr>
<tr>
<td>TUE DEC 5</td>
<td>Partly Cloudy</td>
<td>66°'/48°'</td>
<td>20%</td>
<td>SE 5 mph</td>
<td>62%</td>
</tr>
<tr>
<td>WED DEC 6</td>
<td>Partly Cloudy</td>
<td>68°'/50°'</td>
<td>20%</td>
<td>ESE 7 mph</td>
<td>62%</td>
</tr>
</tbody>
</table>

#### Retrieved on 12/03/2017, 9:28am – 8 days later

<table>
<thead>
<tr>
<th>DAY</th>
<th>DESCRIPTION</th>
<th>HIGH / LOW</th>
<th>PRECIP</th>
<th>WIND</th>
<th>HUMIDITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>TODAY DEC 3</td>
<td>Partly Cloudy</td>
<td>69°'/51°'</td>
<td>10%</td>
<td>SSW 7 mph</td>
<td>76%</td>
</tr>
<tr>
<td>MON DEC 4</td>
<td>Partly Cloudy</td>
<td>73°'/52°'</td>
<td>0%</td>
<td>ENE 18 mph</td>
<td>18%</td>
</tr>
<tr>
<td>TUE DEC 5</td>
<td>Partly Cloudy/Wind</td>
<td>74°'/49°'</td>
<td>0%</td>
<td>NE 23 mph</td>
<td>11%</td>
</tr>
<tr>
<td>WED DEC 6</td>
<td>Sunny</td>
<td>77°'/53°'</td>
<td>0%</td>
<td>NNE 7 mph</td>
<td>16%</td>
</tr>
</tbody>
</table>

The Oil Age: World Oil Production 1859-2050

Rob Bracken, Dave Menninger, Michael Poremba, and Richard Katz - 2006

The Power of Oil

Production and Consumption

World Oil Reserves

The Growing Gap

Oil's Cousins: Coal and Natural Gas

III.2 The Oil Age: World Oil Production 1859-2050 - Rob Bracken, Dave Menninger, Michael Poremba, and Richard Katz - 2006
III. Tectonic Movements and Earthquake Hazard Predictions

Michael W. Hamburger, Chuck Meertens, and Elisha F. Hardy - 2007
Impact of Air Travel on Global Spread of Infectious Diseases

Epidemic spreading pattern changed dramatically after the development of modern transportation systems.

In pre-industrial times disease spread was mainly a spatial diffusion phenomenon. During the spread of Black Death in the 14th century Europe, only few traveling means were available and typical trips were limited to relatively short distances on the time scale of one day. Historical studies confirm that the disease diffused smoothly generating an epidemic front traveling as a continuous wave through the continent at an approximate velocity of 200-400 miles per year.

The central map represents the cumulative number of cases in the world after the first year from the start of a pandemic influenza with $R_0=1.9$ originating in Hanoi (Vietnam) in the Spring.

The US maps focus on the situation in the US after one year, and show the effect of changes in the original scenario analyzed. Different color coding is used for the sake of visualization.

Forecasts of the Next Pandemic Influenza

Forecasts are obtained with a stochastic computational model which explicitly incorporates data on worldwide air travel and detailed census data to simulate the global spread of an influenza pandemic.

The modeling approach considers infection dynamics (i.e., virus transmission, onset of symptoms, infectiousness, recovery, etc.) among individuals living in urban areas around the world, and assumes that individuals are allowed to travel from one city to another by means of the airline transportation network.

Numerical simulations provide results for the temporal and geographic evolution of the pandemic influenza in 3,100 urban areas located in 220 different countries. The model allows to study different spreading scenarios, characterized by different initial outbreak conditions, both geographical and seasonal.

Reproductive Number ($R_0$)

The model includes the worldwide air transportation network (source: IATA) composed of 3,100 airports in 220 countries and $R_0=1.7$, 343 direct connections, each of them associated to the corresponding passenger flow. This dataset accounts for 99% of the worldwide traffic and is complemented by the census data of each large metropolitan area served by the corresponding airport.

Additional spreading scenarios can be obtained by modeling different levels of infectiousness of the virus, as expressed in terms of the reproductive number $R_0$, representing the average number of infections generated by a sick person in a fully susceptible population.

Intervention strategies modeling the use of antiviral drugs can be considered. Two scenarios are compared: an uncooperative strategy in which countries only use their own stockpiles, and a cooperative intervention which simulates a limited worldwide sharing of the resources.
Modeling Advantage

Models are widely used in the construction of scientific theories as they help
• Make assumptions explicit
• Describe the structure and dynamics of systems
• Communicate and explain systems
• Suggest possible interventions
• Identify new questions
Modeling Approaches

- Qualitative and quantitative models
- Deductive, abductive, and inductive models
- Analytic and predictive models
- Universal and domain specific models
- Multi-level (micro-macro) and multi-perspective models
Model Types

- Deterministic models
- Stochastic models
- Epidemic models
- Game-theoretic models
- Network models
- Agent-based models
Models of Science, Technology, and Innovation

STI models use qualitative and quantitative data about scholars, papers, patents, grants, jobs, news, etc. to describe and predict the probable structure and/or dynamics of STI itself.

They are developed in economics, science policy, social science, scientometrics and bibliometrics, information science, physics, and other domains.
Maps of Science & Technology
http://scimaps.org

101st Annual Meeting of the Association of American Geographers, Denver, CO. April 5th - 9th, 2005 (First showing of Places & Spaces)

University of Miami, Miami, FL. September 4 - December 11, 2014.

Duke University, Durham, NC. January 12 - April 10, 2015


100 maps and 12 macroscopes by 215 experts on display at 354 venues in 28 countries.
Examining the Evolution & Distribution of Patent Classifications

Managing Growing Patent Portfolios
Organizations, businesses, and individuals rely on patents to protect their intellectual property and business models. As market competition increases, patenting innovation and intellectual property rights becomes ever more important.

Managing the staggering number of patents demands new tools and methodologies. Grouping patents by their classifications offers an ideal resolution for better understanding how intellectual borders are established and change over time.

The charts below show the annual number of patents granted from January 1, 1976 to December 31, 2002 in the United States Patent and Trademark Office (USPTO) patent archive: slow and fast growing patent classes; the top 10 fast growing patent subclasses; and two evolving patent portfolios.

The Structure and Evolution of the Patent Space
The United States Patent and Trademark Office assigns each patent to one of more than 450 classes covering broad application domains. For example, class 514 encompasses all patents dealing with ‘Drug, Bio-Affecting and Body Treating Compositions.’ Classes are further broken down by subclasses that have hierarchical associations. As one example, class 455 features subclass 99 entitled “with vehicle.”

The top 10 fast growing patent classes for 1998–2002 are listed together with the number of patents granted. Most come from the ‘Computer and Communications’ and the ‘Drugs and Medical’ area.

Patent Portfolio Analysis
A longitudinal analysis of portfolios reveals different patenting strategies. For each year (given in gray above each treemap), a treemap of all new patents granted to the assignees is shown. The number of patents is given below each treemap. The same size and color coding as above was used. In addition, yellow indicates that no patent has been granted in that class in the last 5 years.

Apple Computer, Inc.
Apple Computer, Inc.’s portfolio starts in 1980 and increases considerably in size over time. In most years, more than half of Apple Computer’s patent filings were placed into four classes, namely ‘Information Processing System Organization,’ ‘Computers Graphics Processing, Operator Interface Processing, and Selective Visual Display Systems,’ ‘Image Analysis,’ and ‘Data Processing: Database and File Management or Data Structures.’ These four classes are an integral part of Apple Computer, Inc.’s patent portfolio, receiving patents every year.

Jerome Lemelson
The patent portfolio of Jerome Lemelson shows a very different activity pattern. Starting in 1976, he publishes between 6–20 patents each year. However, the predominance of yellow shows that there is little continuity from previous years in regards to the classes into which patents are filed. No class dominates. Instead, more and more new intellectual space is claimed.

Top-10 Subclasses

<table>
<thead>
<tr>
<th>Class</th>
<th>Title</th>
<th># of Patents</th>
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</thead>
<tbody>
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<td>514</td>
<td>Drug, Bio-Affecting and Body Treating Compositions</td>
<td>18,778</td>
</tr>
<tr>
<td>438</td>
<td>Semiconductor Device Manufacturing Process</td>
<td>17,775</td>
</tr>
<tr>
<td>435</td>
<td>Chemistry: Molecular Biology and Microbiology</td>
<td>17,474</td>
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<tr>
<td>424</td>
<td>Drug, Bio-Affecting and Body Treating Compositions</td>
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<tr>
<td>428</td>
<td>Stock Material or Miscellaneous Articles</td>
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<td>257</td>
<td>Active Solid-State Devices (e.g., Transistors, Solid-State Diodes)</td>
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<td>395</td>
<td>Information Processing System Organization</td>
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<td>359</td>
<td>Optical: Systems and Elements</td>
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<td>365</td>
<td>Static Information Storage and Retrieval</td>
<td>8,392</td>
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<td>Total</td>
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<td>130,910</td>
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WEB OF SCIENCE™ 2016 CITATION LAUREATES

IMPACT OF SCIENTIFIC INNOVATIONS

CHEMISTRY

George Church and Feng Zhang developed application of CRISPR-cas9 gene editing in mouse and human cells.

Dennis Lo Yuk Ming detected cell-free fetal DNA in maternal plasma, a revolution in noninvasive prenatal testing.

Hiroshi Maeda and Yasuhiro Matsumura discovered the enhanced permeability and retention (EPR) effect of macromolecular drugs, a key finding for cancer therapeutics.

PHYSICS

Marvin L. Cohen for theoretical studies of solid materials, prediction of their properties, and especially for the empirical pseudopotential method.

Ronald W.P. Drever, Kip S. Thorne and Rainer Weiss developed the Laser Interferometer Gravitational-Wave Observatory (LIGO) that made possible the detection of gravitational waves.

Celso Grebogi, Edward Ott, and James A. Yorke described a control theory of chaotic systems, the OGY method.

MEDICINE

James P. Allison, Jeffrey A. Bluestone and Craig B. Thompson explained how CD28 and CTLA-4 are regulators of T cell activation, modulating immune response.

Gordon J. Freeman, Tasuku Honjo and Arielle H. Sharpe elucidated programmed cell death-1 (PD-1) and its pathway, which has advanced cancer immunotherapy.

Michael N. Hall, David M. Sabatini and Stuart L. Schreiber discovered the growth regulator Target of Rapamycin (TOR) and the mechanistic Target of Rapamycin (mTOR).

ECONOMICS

Olivier J. Blanchard contributed to macroeconomics, including determinants of economic fluctuations and employment.

Edward P. Lazear developed the distinctive field of personnel economics.

Mark J. Melitz pioneered descriptions of firm heterogeneity and international trade.

Annually, Thomson Reuters analysts mine scientific literature citation data to identify the researchers whose work is worthy of Nobel recognition for induction into the Hall of Citation Laureates. They are the innovators responsible for the world’s most influential scientific discoveries, with scholarly papers typically ranking in the top 0.1% by citations within their field. Many go on to win the Nobel Prize for their significant contributions toward the advancement of science.

To learn more visit: stateofinnovation.com

Source: Thomson Reuters Web of Science, InCites Essential Indicators. Visit stateofinnovation.com to learn more about the 2016 Thomson Reuters Citation Laureates.

http://stateofinnovation.com/2016-citation-laureates
Chemical Research & Development
Powers the U.S. Innovation Engine

Macroeconomic Implications of Public and Private R&D Investments in Chemical Sciences

The Council for Chemical Research (CCR) has provided the U.S. Congress and government policy makers with important results regarding the impact of Federal Research & Development (R&D) investments on U.S. innovation and global competitiveness through its commissioned 5-year two phase study. To take full advantage of typically brief access to policy makers, CCR developed the graphic below as a communication tool that distills the complex data produced by these studies in direct, concise, and clear terms.

The design shows that an input of $1B in federal investment, leveraged by $5B in industry investment, brings new technologies to market and results in $10B of operating income for the chemical industry. $40B of growth in the Gross National Product (GNP) and further impacts the US economy by generating approximately 600,000 jobs, along with a return of $8B in taxes. Additional details, also reported in the CCR studies, are depicted in the map to the left. This map clearly shows the two R&D investment cycles; the shorter industry investment at the innovation stage to commercialization cycle; and the longer federal investment cycle which begins in basic research and culminates in national economic and job growth along with the increase in tax base that in turn is available for investment in basic research.

MEDICAL SPECIALTIES
HAS 72
SUBDISCIPLINES

MAP OF SCIENCE: FORECASTING LARGE TRENDS IN SCIENCE

COLLABORATIVE EFFICIENCY

0.6 0.7 0.8 0.9 1

DISCIPLINARY OUTPUT

SCIENTIFIC COLLABORATIONS BETWEEN WORLD CITIES & COUNTRY WISE
https://www.youtube.com/watch?v=lByX2_eb_QQ
Government, academic, and industry leaders discussed challenges and opportunities associated with using big data, visual analytics, and computational models in STI decision-making.

Conference slides, recordings, and report are available via http://modsti.cns.iu.edu/report
Modelling Challenges

Comprise among others:

- Model utility and usability
- Model credibility and validation
- Model extendibility and reproducibility
- Model sharing and retrieval
Modelling Opportunities

Now available:

• High-quality, high coverage, interlinked data
• Cost-effective storage and computation
• Validated, scalable algorithms
• Visualization and animations capabilities
Modeling and Visualizing Science and Technology Developments
National Academy of Sciences Sackler Colloquium, December 4-5, 2017, Irvine, CA

Rankings and the Efficiency of Institutions
H. Eugene Stanley | Albert-László Barabási | Lada Adamic | Marta González | Kaye Husbands Fealing | Brian Uzzi | John V. Lombardi

Higher Education and the Science & Technology Job Market
Katy Börner | Wendy L. Martinez | Michael Richey | William Rouse | Stasa Milojevic | Rob Rubin | David Krakauer

Innovation Diffusion and Technology Adoption
William Rouse | Donna Cox | Jeff Alstott | Ben Shneiderman | Rahul C. Basole | Scott Stern | Cesar Hidalgo

Modeling Needs, Infrastructures, Standards
Paul Trunfo | Sallie Keller | Andrew L. Russell | Guru Madhavan | Azer Bestavros | Jason Owen-Smith

nasonline.org/Sackler-Visualizing-Science