Statistical Models for Science and Innovation Policy

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“Whether it's improving our health or harnessing clean energy, protecting our security or succeeding in the global economy, our future depends on reaffirming America's role as the world's engine of scientific discovery and technological innovation.”

— President Barack Obama
The public has generally treated this progress as something that just happened, without recognizing that it is, in fact, largely the result of a sustained federal commitment to support science through science policies.”

— http://science-policy.net
Science and Innovation Policy

- Goal: identify administrative, financial, political actions
- Actions chosen to have impact on, e.g.,
  - Stimulating breakthrough research
  - Increasing economic prosperity
  - Broadening participation
- Government, private sector, education
- This talk: statistical models for facilitating efficient, data-driven science policy decisions
Examples of Policy Actions

- **Funding actions:**
  - Using federal funds for research on human stem cells
  - “People not projects” vs. pre-defined deliverables

- **Patenting actions:**
  - Granting software patents

- **Educational actions:**
  - Running high school outreach activities
  - Providing mentoring programs
Data-Driven Policy Decisions

- Discovery: identifying possible policy actions
- Prediction: estimating expected impact
- Evaluation: assessing observed outcomes

⇒ Automated data analysis
“Scientific information is both the basic raw material for, and one of the principal products of, scientific research [...] Scientists find out what other scientists are accomplishing through [...] journals, books, abstracts and indexes, bibliographies, reviews.”

— NSF Brochure, 1962
Approach: Statistical Models

- **Modeling challenges:**
  - Aggregating and representing large data sets
  - Handling data from sources with disparate emphases
  - Reasoning under uncertain information
  - Performing efficient inference

- **Bayesian latent (hidden) variable models:**
  - Powerful and flexible [Wallach et al. & Adams et al., AISTATS '10]
  - This talk: statistical topic models
My Research Goal

To develop new **statistical models** and **computational tools** for representing and analyzing large quantities of **complex data** in order to better enable scientific policy-makers to identify and evaluate **high-impact policy actions** and advance the **study of science and innovation policy**.
Collaborate to Study Collaboration

“There needs to be a greater focus on what these [science interaction] data mean [...] This requires the input of social scientists, rather than just those more traditionally involved in data capture, such as computer scientists.”

— Julia Lane, NSF, 24 March 2010
This Talk

- Background: statistical topic models
- Building “off-the-shelf” statistical topic models
- Finding science-directed research clusters
- Evaluating statistical topic models
- Current and future research directions
This Talk

- Background: statistical topic models
Why Topic Models?

From (9) it can then be shown that (Exercise
\[ \lambda = (K^{-1} - K^{-1}M(M^T K^{-1} M) + K^{-1} M M^T K^{-1} M)^{-1} \]
so that the resulting prediction
\[ \lambda^T Z = k^T Z \]
which is identical to what would result from generalized least squares estimation.

\[ k_u = k^T Z \]
where \( \gamma = m(x_0) - M^T K^{-1} M \)

Best linear unbiased prediction, named after the Sarda 1951; Journel and Huijbregts 1978 process is assumed to be an ordinary prediction is called ordinary. The more general \( m \) is known a with the mean assumed 0 is generally called objective analysis Pedder 1987 and Daley 1991. A linear unbiased prediction for regression model did not explicitly consider the spatial setting. C further discussion on the history of various for.

As noted in 1.3, A useful characterization of

**Definition 2.1** A Gaussian process is a \( \mathcal{C} \) finite number of which have a joint Gaussian

Gaussian process as

\[ f(x) \sim \mathcal{GP}(m(x)) \]

by simplification we will that not be done, see section the random variables represent Gaussian processes are random variables is time. Here the index set \( \mathcal{X} \) is the be more general, e.g. \( \mathbb{R}^D \). For notational enumeration of the cases in the training set such that \( f_i \sim f(x_i) \) is the random variable as would be expected.
Seeking Life’s Bare (Genetic) Necessities

Cold Spring Harbor, New York—How many genes does an organism need to survive? Last week at the genome meeting here, two genome researchers with radically different approaches presented complementary views of the basic genes needed for life. One research team, using computer analyses to compare known genomes, concluded that today’s organisms can be sustained with just 250 genes, and that the earliest life forms required a mere 128 genes. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn’t be enough.

Although the numbers don’t match precisely, those predictions “are not all that far apart,” especially in comparison to the 75,000 genes in the human genome, notes Siv Andersson of Uppsala University in Sweden, who arrived at the 800 number. But coming up with a consensus answer may be more than just a genetic numbers game, particularly as more and more genomes are completely mapped and sequenced. “It may be a way of organizing any newly sequenced genome,” explains Arcady Mushegan, a computational molecular biologist at the National Center for Biotechnology Information (NCBI) in Bethesda, Maryland. Comparing an


Stripping down. Computer analysis yields an estimate of the minimum modern and ancient genomes.
Generative Statistical Modeling

- Assume data was generated by a probabilistic model:
  - Model may have hidden structure (latent variables)
  - Model defines a joint distribution over all variables
  - Model parameters are unknown
- Infer hidden structure and model parameters from data
- Situate new data into estimated model
Directed Graphical Models

\[ P(y, x_1, \ldots, x_N) = P(y) \prod_{n=1}^{N} P(x_n | y) \]

- Nodes: random variables (latent or observed)
- Edges: probabilistic dependencies between variables
- Plates: “macros” that allow subgraphs to be replicated
Statistical Topic Modeling

\[ \begin{align*}
  \theta_d & \rightarrow Z_n \\
  Z_n & \rightarrow W_n \\
  W_n & \rightarrow \phi_t \\
  D & \rightarrow N \\
  N & \rightarrow T \\
  \text{document-specific topic distribution} & \rightarrow \text{observed word} \\
  \text{topic assignment} & \rightarrow \text{topics}
\end{align*} \]

[Hofmann, '99]
Latent Dirichlet Allocation (LDA)

[Blei, Ng & Jordan, '03]
The State of The Art

- Topic models are extremely popular
- ... but they're not always usable by non-experts
- Need to bridge this gap between producers and consumers of topic modeling technology:
  - Address problems/challenges faced by practitioners
  - Question unquestioned assumptions
  - Explore the interplay between theory and practice
This Talk

- Background: statistical topic models
- Building “off-the-shelf” statistical topic models

[Wallach et al., NIPS '09]

Collaborators: Sarah Kaplan, Rotman, University of Toronto; Andrew McCallum, UMass Amherst; David Mimno, UMass Amherst
“Off-the-Shelf” Topic Modeling

I want to model technology emergence by analyzing patent abstracts...

I have a statistical model that you can use...
"Off-the-Shelf" Topic Modeling

I want to model technology emergence by analyzing patent abstracts...

I have a statistical model that you can use...

| a field emission an electron ... | a the carbon and gas ... | the of a to and ... | the invention of to present ... |
“Off-the-Shelf” Topic Modeling?

Help! All my topics consist of “the, and of, to, a ...”

Now they all consist of “invention, present, thereof ...”

Wait, but how do I choose the right number of topics?

Preprocess your data to remove stop words...

Make a domain-specific list of stop words...

Evaluate the probability of unseen data for different numbers...
Discrete Probability Distributions

- 3-dimensional discrete probability distributions can be visually represented in 2-dimensional space:
Dirichlet Distribution

- Distribution over discrete probability distributions:

\[ p \sim \text{Dir}(\alpha m) \]
Dirichlet Parameters

\[ m = \left( \frac{5}{7}, \frac{1}{7}, \frac{1}{7} \right) \]

\[ m = \left( \frac{1}{7}, \frac{5}{7}, \frac{1}{7} \right) \]

\[ m = \left( \frac{1}{7}, \frac{1}{7}, \frac{5}{7} \right) \]

\[ m = u = \left( \frac{1}{3}, \frac{1}{3}, \frac{1}{3} \right) \]

\[ \alpha = 3 \]  \quad \alpha = 6 \quad \alpha = 30 \]
Dirichlet Priors for LDA

symmetric priors: uniform base measures
Dirichlet Priors for LDA

- Two scalar concentration parameters: $\alpha$ and $\beta$
- Concentration parameters are usually set heuristically
  - e.g., $\alpha = 50$ and $\beta = 0.01W$
- Some recent work on learning optimal values for the concentration parameters from data
- No rigorous study of the Dirichlet priors:
  - e.g., asymmetric vs. symmetric base measures
  - Effects of the base measures on the inferred topics
Symmetric $\rightarrow$ Asymmetric

- Use prior over $\Theta = \{\theta_1, \ldots, \theta_D\}$ as a running example
- Uniform base measure $\rightarrow$ nonuniform base measure

$$\Theta \sim \text{Dir}(\alpha m) \quad \Theta \sim \text{Dir}(\alpha m)$$

- Asymmetric prior: some topics more likely a priori
Hierarchical Asymmetric Dirichlet

- Which topics should be more probable a priori?
  - Draw $m$ from a Dirichlet distribution:
Symmetric Dirichlet is a special case of the hierarchical asymmetric Dirichlet (large concentration parameter)
Putting Everything Together

- Asymmetric hierarchical Dirichlet priors
- Integrate out $\Theta$, $\Phi$ and base measures
- Learn $z$ and concentration parameters from data
Data Sets

● Carbon nanotechnology patents:
  - Ultimate goal: track innovation and emergence
  - Fullerene and carbon nanotube patents
  - 1,016 abstracts (~100 words each)
  - 103,499 words
  - 6,068 unique words
● 20 Newsgroups data (80,012 total words)
● New York Times articles (477,465 total words)
<table>
<thead>
<tr>
<th>before</th>
<th>after</th>
</tr>
</thead>
<tbody>
<tr>
<td>a field emission an electron ...</td>
<td>the invention of to present ...</td>
</tr>
<tr>
<td>a the carbon and gas ...</td>
<td>the of a to and ...</td>
</tr>
<tr>
<td>the of</td>
<td>metal catalytic transition catalyst from ...</td>
</tr>
<tr>
<td>a of to and ...</td>
<td>composite polymer matrix weight fiber ...</td>
</tr>
<tr>
<td>a carbon nanotubes catalyst substrate ...</td>
<td>metal catalytic transition catalyst from ...</td>
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<tr>
<td>the of</td>
<td>metal catalytic transition catalyst from ...</td>
</tr>
<tr>
<td>the invention</td>
<td>the invention of to present ...</td>
</tr>
</tbody>
</table>
Sampled Concentration Parameters

\[ \alpha', \alpha, \beta, \log\beta' \]

\[ \theta_d \rightarrow z_n \rightarrow w_n \rightarrow \phi_t \]

\[ D \rightarrow \mathcal{N} \rightarrow \mathcal{T} \]
Sampled Concentration Parameters
Intuition

- Topics should be distinct from each other:
  - Asymmetric prior over topics makes topics more similar to each other (and to corpus-wide word frequencies)
  - Want a symmetric prior to preserve topic “distinctness”

- Still have to account for power-law word usage:
  - Asymmetric prior over document-specific topic distributions means some topics (e.g., “the, a, of, to ...”) can be used more often than others in all documents
Number of Topics

symmetric

asymmetric
"Off-the-Shelf" Topic Modeling

I can model technology emergence by analyzing patent abstracts!

Great! Let me know if you need any more help!

<table>
<thead>
<tr>
<th>the</th>
<th>carbon nanotubes</th>
<th>metal catalytic transition catalyst</th>
<th>composite polymer matrix weight fiber</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
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<td>from</td>
<td>weight fiber</td>
</tr>
<tr>
<td>of</td>
<td>substrate</td>
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<td></td>
</tr>
<tr>
<td>to</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>and</td>
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<td>...</td>
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</tr>
</tbody>
</table>
Declining Topics
Rising Topics

![Graph showing trends in carbon nanotube transistors and carbon nanotube electronics from 1991 to 2004. The graph indicates a significant increase in interest in carbon nanotube transistors around 1997, followed by a steady increase until 2004. Carbon nanotube electronics also show an increase in interest, particularly after 2000.](image-url)
Building Other Tools

- **Topic-based language modeling** [Wallach, ICML '06]
  - Predict the next word given previous words
  - Topics can provide useful information
  - Have to model stop words

- **Polylingual topic modeling** [Mimno et al., EMNLP '09]
  - Track scientific progress in other countries
  - Simultaneously model text in many languages
  - Need robustness to word usage in many languages
This Talk

- Background: statistical topic models
- Building “off-the-shelf” statistical topic models
- Finding science-directed research clusters

[Wallach, Ph.D. Thesis '08]

Collaborators: Ned Talley, NIH; Mark Boguski, Harvard Medical School Library
National Institutes of Health

- NIH funds biomedical and health-related research
- 27 institutes and centers:
  - Often disease-focused (e.g., cancer, diabetes)
  - ... but complicated by politics and expediency
  - Diseases cross scientific boundaries
  - Overlap in the research funded
- Daunting landscape for choosing research directions, funding allocations, and policy actions
Finding Science-Directed Clusters

• Lots of information redundancy between institutes
• Goal: characterize redundancy and overlap
  – To what extent do science-directed clusters correspond with institute categorizations?
• Approach: unsupervised content-based clustering
  – Assign each proposal to a single cluster
  – Learn the most appropriate number of clusters
• Cluster by topic not raw word usage
NIH Grant Proposals

- 60,568 grant proposals funded by NIH in 2007
- Proposals arranged according to document similarity using a force-directed layout algorithm
- Areas are hand-labeled
- Familiar representation
Cluster-Based Topic Modeling

document-specific cluster indicator

cluster-specific Dirichlet
“Patient-Oriented Services”

- health
- public
- research
- african
- ...

- patients
- disease
- treatment
- clinical
- ...

- social
- behavior
- behavioral
- behaviors
- ...

- data
- methods
- models
- analysis
- ...

NIMH
NIDA
NCI
NICHD
NIA
“Cellular and Molecular Biology”

membrane proteins assembly fusion ...

mechanisms molecular understanding studies ...

screening high small throughput ...

proteins protein function complex ...

NIGMS NIAID NCI NINDS NIDDK
“Biology of Dividing Cells”

<table>
<thead>
<tr>
<th>cell</th>
<th>mechanism</th>
<th>proteins</th>
<th>function</th>
</tr>
</thead>
<tbody>
<tr>
<td>cells</td>
<td>molecular</td>
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</tr>
<tr>
<td>apoptosis</td>
<td>understanding</td>
<td>function</td>
<td>increased</td>
</tr>
<tr>
<td>growth</td>
<td>studies</td>
<td>complex</td>
<td>effects</td>
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- Evaluating statistical topic models

[Wallach et al., ICML '09]

Collaborators: David Mimno, UMass Amherst; Iain Murray, University of Edinburgh; Ruslan Salakhutdinov, MIT; Ned Talley, NIH
Evaluating Topic Models

- Topic models are unsupervised so evaluation is hard
- A lot of topic modeling research has skirted this issue
- Easy to get a sense of topics from “eyeballing” output
  - ... but this isn't rigorous evaluation
- Existing methods for computing probability of held-out documents are inaccurate [Wallach et al., ICML '09]
  - Proposed 2 new, accurate methods
- Also need expert-driven evaluation
Expert-Driven Evaluation

● Scientific policy-makers know their own domains

● Invaluable resource for model evaluation:
  - Identification of good/poor quality topics
  - Characterization of different types of topics

● Collaborative research:
  - Automated evaluation metrics
  - Prior distributions that influence model output
Evaluation of NIH Topics

- 2 experts from NIH, 150 topics (NINDS coverage)
- Collaboratively developed 3-stage evaluation protocol
- 4 classes of poor quality topics:
  - Intruded: 2 or more unrelated concepts
  - Chained: e.g., “fatty acids” → “acids” → “nucleic acids”
  - Unbalanced: mix of general and specific terms
  - Random: no clear concept represented
Evaluation Metrics

- Number of words assigned to each topic (topic size)
- Within-document co-occurrence of the top words

<table>
<thead>
<tr>
<th>Intruded</th>
<th>Chained</th>
</tr>
</thead>
<tbody>
<tr>
<td>sleep</td>
<td>cerebellar</td>
</tr>
<tr>
<td>sars</td>
<td>cerebellum</td>
</tr>
<tr>
<td>insomnia</td>
<td>pb</td>
</tr>
<tr>
<td>cov</td>
<td>purkinje</td>
</tr>
<tr>
<td>disturbances</td>
<td>ag</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
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<td>disturbances</td>
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</tr>
<tr>
<td>...</td>
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```
<table>
<thead>
<tr>
<th>Word</th>
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<td>2</td>
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<tr>
<td>purkinje</td>
<td>318</td>
<td>228</td>
</tr>
<tr>
<td>ag</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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Automated Evaluation

- Word co-occurrence-based metric:
  - 17 of 20 worst-scoring topics are “bad”
  - 18 of 20 best-scoring topics are “good”

- Goal: incorporate co-occurrence information into the prior over topic-specific word distributions:
  - Words that do not co-occur should not have high probability within the same topic
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Diversity of Science

- Policy actions shape the diversity of science:
  - Idea diversity: array of different ideas
  - Individual diversity: variety of people and organizations
- Goal: develop new methods and tools for:
  - Quantifying the diversity of science
  - Assessing impact of policy actions on diversity

Collaborators include: Fiona Murray, Sloan School, MIT
Software Development Communities

- Free & open source software (FOSS):
  - Complex technological, legal, social structures
  - Collaboration on a massive scale
- Most communication is online and publicly available
  - Informal documents: messy, unstructured
- Goal: use these data to study organizational and social processes underlying FOSS development

Collaborators include: Benjamin Mako Hill, Sloan School, MIT; openhatch.org
Thanks!

Acknowledgements: Mark Boguski, Harvard Medical School Library; Sarah Kaplan, Rotman, University of Toronto; Andrew McCallum, UMass Amherst; David Mimno, UMass Amherst; Iain Murray, University of Edinburgh; Ned Talley, NIH; Ruslan Salakhutdinov
Cross-language Analysis

“He may know one language backwards and forward, but he can't communicate with a scientist who only knows another: a graphic illustration of the need for translation of foreign scientific documents.”

— NSF Brochure, 1962
Polylingual Topics

| CY | sadwrn blaned gallair at lloeren mytheleg |
| DE | space nasa sojus flug mission           |
| EL | διαστημικό sts nasa αγγι small       |
| EN | space mission launch satellite nasa spacecraft |
| FA | فضایی ماموریت ناسا مدار فضانورد ماهواره |
| FI | sojuz nasa apollo ensimmäinen space lento |
| FR | spatiale mission orbite mars satellite spatial |
| HE | התלולים הארצים חלול כדי א תוכנין |
| IT | spaziale missione programma space sojuz stazione |
| PL | misja kosmicznej stacji misji space nasa |
| RU | космический союз космического спутник станции |
| TR | uzay soyuz ay uzaya salyut sovyetler |
Polylingual Topics

<table>
<thead>
<tr>
<th>Code</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>CY</td>
<td>bardd gerddi iaith beirdd fardd gymraeg</td>
</tr>
<tr>
<td>DE</td>
<td>dichter schriftsteller literatur gedichte gedicht werk</td>
</tr>
<tr>
<td>EL</td>
<td>ποιητής ποίηση ποιητή έργο ποιητές ποιήματα</td>
</tr>
<tr>
<td>EN</td>
<td>poet poetry literature literary poems poem</td>
</tr>
<tr>
<td>FA</td>
<td>شاعر شعر ادبیات فارسی ادبی آثار</td>
</tr>
<tr>
<td>FI</td>
<td>runoilija kirjailija kirjallisuuden kirjoitti runo julkaisi</td>
</tr>
<tr>
<td>FR</td>
<td>poète écrivain littérature poésie littéraire ses</td>
</tr>
<tr>
<td>HE</td>
<td>משורר ספרות שירה ספרشور השירים</td>
</tr>
<tr>
<td>IT</td>
<td>poeta letteratura poesia opere versi poema</td>
</tr>
<tr>
<td>PL</td>
<td>poeta literatury poezji pisarz in jego</td>
</tr>
<tr>
<td>RU</td>
<td>поэт его писатель литературы поэзии драматург</td>
</tr>
<tr>
<td>TR</td>
<td>şair edebiyat şiir yazar edebiyatı adlı</td>
</tr>
</tbody>
</table>
Aligned Corpora

- Fully parallel corpora: direct translations
  - Expensive to produce, relatively rare
- Partially parallel corpora: few parallel “glue” tuples
  - < 25% is sufficient to obtain aligned topics
- Comparable corpora: documents have similar content
  - e.g., Wikipedia in English, Farsi, Finnish, French, German, Greek, Hebrew, Italian, Polish, Russian, Turkish, Welsh
  - e.g., patent–paper pairs (legal vs. scientific language)
Polylingual Topic Model

“tuple” of aligned documents

language-specific Dirichlet parameters
Differences in Topic Emphasis

world
ski
km
won
...

ottoman
empire
khan
byzantine
...

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Held-Out Log Probability

- Classic way to evaluate probabilistic generative models
- Involves an intractable sum for topic models

$P(\text{data} | \text{model})$  

higher is better
An Empirical Comparison