Topic Modeling for Scientific Documents

Jethro Kuan
WING-NUS

Abstract

Topic models are statistical models, used to discover abstract topics that occur in a collection of documents. In this paper, we focus on the technique of topic modeling, particularly in its application to the domain of scientific documents. We discuss different approaches to topic modeling, and weigh in on their strengths and shortcomings.

1 Introduction

In this information age, the availability of knowledge is insufficiently met with the tools to navigate it. Tools like Semantic Scholar use machine learning to process scientific documents and extract meaningful structure, empowering researchers to discover papers more relevant to their work. One such technique is topic modeling.

Topic modeling attempts to discover abstract topics within documents. Most topic models are generative models, assuming that latent variables govern the generative process of a document. A document is often modeled to be produced from a distribution of topics, and topics themselves are distributions over the vocabulary of the corpora.

A topic model trained on a corpora of scientific documents could learn topics such as "Neural Networks", "Biology" and "Medicine". Topics attribute a high probability to words that relate to the topic. For example, a "Neural Networks" topic would give attribute a high probability to "classifiers", and a low probability to "bacteria". The quotations around the topics are to make explicit that the labels are human interpretations of what these topics may be. Topic modeling is an unsupervised problem, and is often trained on unlabeled data. Automatic labeling of these topics is an active area of research [6], [5].

Topic modeling may discover that document in Figure 1 relates to "Medicine" and "Neural Networks", because these topics give rise to the colored words in the document.

In addition, we can view these abstract topics as a form of clustering. Researchers are better able to navigate the large corpora of scientific knowledge, by exploring documents that have similar topic proportions.

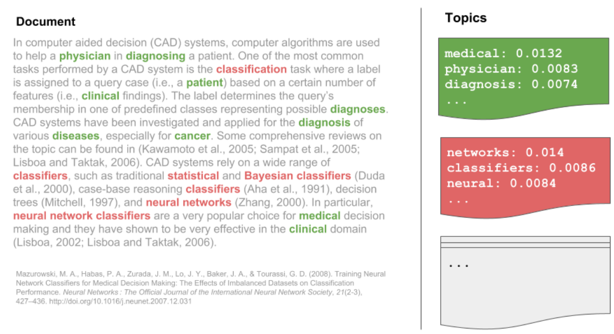

Figure 1: According to the trained topic model, topics like "Medicine" and "Neural Networks" generate the colored words of the document

In this paper, we briefly discuss the predominant model: Latent Dirichlet Allocation (LDA) and its variants. In addition, we explore other models that are not derivatives of LDA, such as the Replicated Softmax.

2 LDA

Latent Dirichlet analysis is widely considered to be the simplest topic model. LDA models each document as a mixture of topics, where a topic β_k is a probability distribution over a fixed vocabulary of terms. Training LDA requires fixing the number of topics, K. We can draw the graphical model for LDA as in Figure 2.

At risk of being pedantic, we explain the graphical model in detail. η is the topic hyperparameter, which produces a topic distribution β_k of the Dirichlet family. There are a total of K topics. Similarly, α is a hyperparameter that produces the per-document topic proportions θ_d. These Dirichlet distributions are of dimension $K-1$, because there are a total of K topics. There are D such topic proportions, where D is the total number of documents. $Z_{d,n}$ is the per-word topic assignment, drawn from the particular θ_d. Finally, $W_{d,n}$ is the nth word in the dth document, an observed variable. It is simple to see that $P(W_{d,n}|Z_{d,n}, \beta_k) = \beta_{z_{d,n}, w_{d,n}}$.

A high α value encodes the belief that documents contain a mixture of many topics, rather than being largely represented by a few topics. Similarly, a high η value encodes the belief that topics has high probability for a large number of words in the vocabulary.

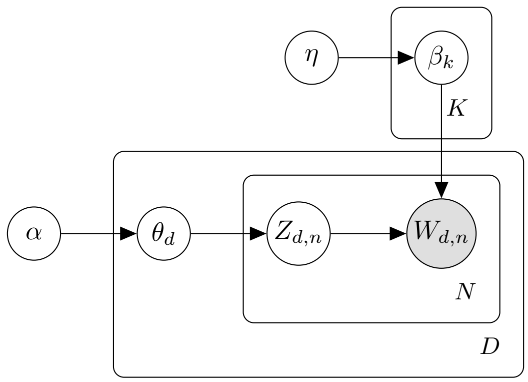

Figure 2: Plate notation for LDA, a directed graphical model.

We can fully specify the model, by looking at the joint distribution $\mathcal{J}$ of all the latent and observed variables.

$$\mathcal{J} = \left(\sum_{k=1}^{K} P(\beta_k|\eta)\right)\left(\sum_{d=1}^{D} P(\theta_d|\alpha)\right) \left(\sum_{n=1}^{N} \theta_{d,Z_{d,n}}\beta_{Z_{d,n},W_{d,n}}\right) \quad (1)$$

The generative process of a document is as follows:

Algorithm 1 Generative Process of LDA

for each document d in D **do**
  Draw topic distribution $\theta_d \sim Dir(\alpha)$
  for each word n_d in N_d **do**
    Sample topic $z_{d,n} \sim Multinomial(\theta)$
    Sample word $w_{d,n} \sim Multinomial(\beta_{z_{d,n}})$

If we fix the topic distributions $\beta_{1:K}$, we can compute the per-document posterior θ given the document.

$$P(\theta|w_{1:n}, \alpha, \beta_{1:K}) = \frac{P(\theta|\alpha)\prod_{n=1}^{N} P(z_n|\theta)P(w_n|z_n, \beta_{1:K})}{\int_\theta P(\theta|\alpha)\prod_{n=1}^{N}\sum_{z=1}^{K} P(z_n|\theta)P(w_n|z_n, \beta_{1:K})} \quad (2)$$

The denominator is intractable to compute, due to the coupling between θ and β under the multinomial assumption. [3]. Hence, we rely on techniques for approximate inference of the posterior. We discuss these techniques in section 4.

Why does LDA work? The Dirichlet distribution encourages sparsity, encoding the belief that the document-topic distribution has few topics per document, and the topic-word distribution has few words per topic. These two beliefs work against each other, and LDA discovers this sparsity balance, which gives rise to the structure of the textual data.

2.1 Statistical Assumptions

As Mackay quips, we cannot make inference without statistical assumptions. LDA makes several assumptions, some rendering it less suited for application to the domain of scientific documents.

LDA models documents as "bag-of-words": words within the document are interchangeable. [3] I think this is a reasonable assumption to make, given the task is to discover themes within the document.

LDA also assumes that the order of documents do not matter. Exchangeability of both words and documents allows LDA to model the joint distribution as a mixture model. I believe this assumption to be invalid in the domain of scientific documents. The meaning of keyphrases used in scientific literature change over time. For example, the landscape of research neural networks is vastly different now, as compared to the 1990s, and LDA will fail to capture these differences.

Variants of LDA relax these statistical assumptions, or make other assumptions in place. We discuss Dynamic Topic Modeling (DTM) in section 3, and briefly mention the rest in the appendix.

3 Dynamic Topic Modeling

Dynamic Topic Modeling (DTM) was proposed to remove the assumption that documents are *exchangeable.* [2]

The order of documents are important for scientific documents, since both the content, and the meaning of words evolve over time.

In DTM, data is divided by discrete time slices. The topics associated with time slice t evolve from the time slice $t-1$. Because the Dirichlet distribution is not amenable to sequential modeling, we use the Gaussian distribution to model the sequence of random variables.

The generative process for time slice t is as follows:

Algorithm 2 Generative Process of DTM

Draw topic distribution $\beta_t|\beta_{t-1} \sim N(\beta_{t-1}, \sigma^2 I)$
Draw $\alpha_t|\alpha_{t-1} \sim N\left(\alpha_{t-1}, \delta^2 I\right)$
for each document w **do**
  Draw $\eta_{w,t} \sim N\left(\alpha_t, a^2 I\right)$
  for each word at position n **do**
    Sample topic $z_{t,n} \sim Multinomial(\pi(\eta_{w,t}))$
    Sample word $w_{t,d,n} \sim Multinomial(\beta_{t,z,n})$

π maps the multinomial parameters to the mean parameters, $\pi\left(\beta_{k,t}\right)_w = \frac{exp(\beta_{k,t,w})}{\sum_w exp(\beta_{k,t,w})}$

The Multinomial and Guassian distributions are not conjugates, inference via Gibbs sampling is difficult. Hence, variational inference instead.

Further extensions of this approach include the continuous Dynamic Topic Models (cDTM), which removes the discretization of the time slices. [7] This model has been used to predict the timestamp of documents.

4 Inference Methods

Approximating intractable probability densities is a well-studied problem in modern statistics. This problem arises often in Bayesian statistics, where computing posterior probablity densities in requires inference over latent variables. Many learning algorithms have been developed, including collapsed Gibbs Sampling, Variational Inference, Collapsed Variational Inference, and MAP estimation. Each of these approximation techniques have their own strength and shortcomings.

The two inference methods are briefly discussed below, and a comparison between them relegated to the appendix in subsection 4.3.

4.1 MCMC Sampling

Historically, Markov Chain Monte Carlo (MCMC) sampling has been the dominant technique for approximating posterior densities. In MCMC, we construct an ergodic Markov chain on the latent variable z, whose stationary distribution is the posterior $P(z|x)$. Samples are drawn from the stationary distribution, and used to approximate the posterior empirically.

In Gibbs sampling, the space of the Markov Chain is the space of the configurations of the hidden variables. In Gibbs sampling, the next state is reached by sequentially sampling all variables from the distribution, conditioned on all the current sampled values. After a "burn-in" period, the samples would be drawn from the posterior distribution.

Algorithm 3 Gibbs Sampling

1: $x^0 \leftarrow q(x)$
2: **for** $i = 1, 2, 3, \ldots$ **do**
3: **for** $d = 1, 2, 3, \ldots, D$ **do**
4: $x_d^i \sim P(X_1 = x_1 | X_k = x_k^{i-1}$ for $k = \{1..n \setminus d\})$

A full treatment of Gibbs Sampling applied to LDA can be found in [4].

4.2 Variational Inference

Mean field variational inference (MFVI) breaks the coupling between θ and z by introducing free variational parameters γ over θ and ϕ over z and dropping the edges between them. This results in an approximate posterior $q(\theta, z|\gamma, \phi) = q_\gamma(\theta) \prod_n q_\phi(z_n)$.

To best approximate the true posterior, we frame it as an optimization problem, minimizing L where:

$$L(\gamma, \phi|\alpha, \beta) = D_{KL}\left[q(\theta, z|\gamma, \phi)||p(\theta, z|\alpha, \beta)\right] - \log p(w|\alpha, \beta) \tag{3}$$

This optimization has closed form coordinate descent equations for LDA, because the Dirichlet is conjugate to the Multinomial distribution. This computational convenience comes at the expense of robustness, making it difficult to apply to other more complicated topic models.

4.3 Choosing an Inference Method

How do we know which technique to use to approximate the posterior density? MCMC methods are computationally more intensive, but provide samples that are approximately exact from the target posterior density. In contrast, VI methods view the problem as an optimization problem, which allows it to utilize efficient learning algorithms such as stochastic optimization. This is much quicker to compute, and is suited for larger datasets.

MCMC methods, however, cover a large family of sampling methods. Gibbs sampling requires that the prior and posterior are conjugate distributions. When this is not possible, such as in DTM, VI methods can perform better than other methods in the MCMC family.

A closer look at the different inference approximation algorithms, however, shows that the performance differences can be explained away by setting certain smoothing hyperparameters [1].

5 Appendix

5.1 Alternatives to LDA

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