Latent Dirichlet Allocation for scientific topic extraction

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Abstract

We experiment with an automated topic extraction algorithm based on a generative graphical model. Latent Dirichlet Allocation assumes that individual words that appear in a document collection are drawn from a family of distributions associated with a fixed number of topics. We learn these word-topic distributions from a collection of 20000 physics journal articles: the contents of the `arXiv.org/quant-ph` preprint archive between the years 1994 and 2007. We evaluate our results using the perplexity measure on the document collection and report on running time for various settings.

keywords: LDA, topic model, Gibbs sampling, clustering

1 Introduction

There is a growing amount of unstructured data becoming freely available on the web and through various digitization efforts. Due to the enormous scale of these data collections it is unrealistic to assume that human supervision can play any significant role in their classification and curatorship. Clearly, automated largely-unsupervised machine learning techniques will be required in order to deal with the information overload.

The subjects of classification, retrieval and browsing have been central topics of research in the data mining community for the past decade, but there is still more work to be done. Recently, there has been a surge of interest in the machine learning community about "topic models" which attempt to automatically extract the subject matter from document collections [BNJ03, BL09]. These techniques are scalable to very large document collections and produce very informative results despite using the same old data mining paradigm of documents as bags of words.

For this project we will focus our attention on the *latent Dirichlet allocation* (LDA) model which is described in the seminal paper by Blei, Ng and Jordan [BNJ03]. We will use a Gibbs sampling approach to learn the LDA parameters which is very computationally efficient [GS04]. Computational efficiency will be important since our data set contains roughly 20k documents which are represented as word counts of over a dictionary of 10k words.

This report is structured as follows. In the next section we will provide some theoretical background on the LDA model. Afterwards, we will discuss the inference procedure we used to learn the model parameters. Section 4 is describes our data set and the preprocessing we performed. We describe the results of two experiments in section 5 and follow up with some discussion and a conclusion.

2 The model

Latent Dirichlet Allocation is a recent graphical model that has received a lot of attention in the machine learning community. According to the authors, LDA is an evolution of pLSA (probabilistic latent semantic indexing) which allows for documents to have multiple topics [BNJ03].

The generative process associated with LDA is as follows:

1. Pick a document size N_d
2. Pick a set of topics $\theta \sim Dirichlet(\alpha)$
3. For each of the N_d words in document j:
   (a) Choose a topic $z_w \sim Multinomial(\theta)$
   (b) Choose a word w from a topic distibution $p(w|z_w, \varphi)$, a multinomial over words given the topic.

The key thing to note here is that each document can be associated with multiple topics. This feature gives LDA its great power to model real world document collections accurately.

To further understand the generative process consider the plate notation in Fig 1, which shows the dependence relationships. We assume there is a total of T topics, D documents and that the length of each document is N_d.

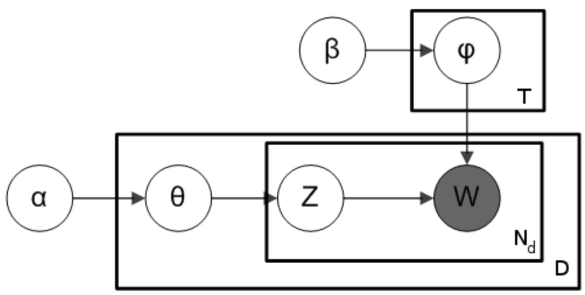

Figure 1: The graphical model behind LDA. θ is the distribution of topics for a document, φ is the distribution of words for a given topic.

Reading the conditional independence relationships that the graph represents we can write the full probability equation as follows:

$$P(\mathbf{W}, \mathbf{Z}, \theta, \varphi; \alpha, \beta) = \prod_{k=1}^{T} P(\varphi_k; \beta) \prod_{j=1}^{D} P(\theta_j; \alpha) \prod_{w=1}^{N_d} P(Z_{j,w}|\theta_j) P(W_{j,w}|\varphi_{Z_{j,w}}), \quad (1)$$

where $P(Z_{j,w}|\theta_j)$ represents the probabilty of picking topic Z for word w in the document j given the topic proportion for document j is θ_j. The other important factor is $P(W_{j,w}|\varphi_{Z_{j,w}})$ which represents the probability of picking word W for the wth word in document j assuming we were drawing it from the topic distribution for topic $Z_{j,w}$.

The notation can be a bit confusing, so it is important to restate the problem in several different ways. Since we are dealing with discrete probability distributions, we can represent them as probability tables.

The table for the φ_{wk} distribution will be of size WxT. Selecting a topic k is equivalent to picking the kth column from the matrix φ_{wk}. I.e. φ_{wk} is a family of K distributions over W words. As for θ_{kj}, we can think of it as a TxD matrix which specifies what is the probability of each topic k to be present in document j.

Of course, real documents are not generated in this manner, so how can this model be useful. It turn out that if we assume such a model is at work, we can infer the parameters of the two distributions φ_{wk} and θ_{kj}, which in turn allows us to classify the documents according to the topics they exhibit.

3 The inference algorithm

First we being by defining some quantities. We have the document set $\mathcal{D} = \{d_1, d_2, \ldots, d_D\}$, where each document consists of a word count vector for the words taken from a fixed vocabulary $\mathcal{W}$ of size W.

$$\begin{aligned}
\gamma_{wjk} &= Pr(z = k|x = w, d = j) = \text{prob. that word } w \text{ in doc } j \text{ comes from topic k.}\\
N_{wj} &= \#\text{ of times } w \text{ appears in doc } j.\\
N_{wk} &= \sum_{j\in\mathcal{D}} N_{wj}\gamma_{wjk} = \#\text{ of times } w \text{ appears in topic } k.\\
N_{kj} &= \sum_{w\in\mathcal{W}} N_{wj}\gamma_{wjk} = \#\text{ of times topic } k \text{ appears in doc } j.\\
N_k &= \sum_{w\in\mathcal{W}} N_{wk} = \sum_{w\in\mathcal{W}}\sum_{j\in\mathcal{D}} N_{wj}\gamma_{wjk} = \#\text{ words assigned to topic } k.\\
N_j &= \sum_{k\in\mathcal{T}} N_{kj} = \sum_{k\in\mathcal{T}}\sum_{w\in\mathcal{W}} N_{wj}\gamma_{wjk} = \#\text{ words in doc } j.
\end{aligned}$$

Our aim is to infer a set of topics $\mathcal{T}$ where each topic is a probability distribution over words $\mathcal{W}$ and at the same time indicate which topics are present in each document. To achieve this we will have to learn the parameters of the two matrices φ_{wk} and θ_{kj} respectively.

There are several approaches for approximate inference and the learning of these distribution: Variational Bayes, Gibbs sampling, collapsed variational Bayes, etc. In a recent paper from ICML09 [AWST] it is shown that all the different models of learning the LDA parameters are actually equivalent and only differ by the setting of the hyper-parameters.

I originally tried to implement the Collapsed Variational Bayes technique of [TNW07], but failed miserably since I had to build in memory the matrix γ_{wjk} which is of size WxDxT. Anyone interested in following this route should consider the wonderful source code by David Andrzejewski [And].

I then chose to use the Gibbs sampling approach [GS04] which can be performed with this code [New]. In order to do Gibbs sampling we need to be able to sample from the conditional distribution of the model. This is by design possible with the probability distibutions associated with the LDA model since they can be expressd in terms of the counts defined above:

$$P(Z_{ij} = k|\mathbf{Z}^{-ij}, x_{ij} = w;\ \alpha, \beta) \quad \propto \quad \left(N_{kj}^{-ij} + \alpha\right) \frac{N_{wk}^{-ij} + \beta}{N_k^{-ij} + W\beta} \tag{2}$$

where the quantity $?^{-ij}$ refers to the same quantity as ? with the contribution of the ith word in the jth document removed. Note that the only calculations that need to be performed are related to the counts N_{wj}, N_{wk}, etc... and so the whole computation is very fast.

I decided to follow the first rule of software development[1] and not try to rewrite Dave Newman's code, but rather use it as a black box. I did read it line by line in order to understand how it works, but it did not make sense to me to try to re-implement the same routines.

4 The data set

The good people who run the arXiv.org were kind enough to send me the entire collection of papers in the `quant-ph` repository! The arXiv is a prominent publication in the physical sciences and contains pre-print versions of most of the important research in several areas. Of particular interest is the field of quantum information science which is very well represented there.

The raw data that was received consists of two directories. The first directory, `pdf/` of size 7.1GB contains 31739 pdf documents. The second directory `tex/` contains the LaTeX source code of some of the papers (its size is 2.1G and it contains 21061 files). Since the source code of only about 2/3 of the papers was available, we decided to use the pdf version of the document collection.

Some more information about the raw dataset.

- Total number of pdf files: 31739
- Total number of papers: 20166 (after removing multiple versions v1,v2)
- Number of files with unreadable/foreign fonts: 6
- Earliest date: 22 Dec 1994 (pdf/9412/9412002v1.pdf)
- Most recent: 30 Mar 2007 (pdf/0703/0703278v1.pdf)

4.1 Textual pre-processing

Since the intended feature vectors are word counts, we used the command-line utility `pdftotext` (part of `xpdf`) to convert the pdf documents to text files. The python script `preprocessing/pdftotext.py` accomplishes this and stores the output in the folder `data/text` while at the same time creating an inventory of all the available documents. At this stage, some documents were found to be unreadable or used foreign language fonts which were not recognized by xpdf. There were very few such documents so it was possible to manually remove them from the inventory.

At this point we had 31732 documents in our "inventory", but some of these documents were different version of the same underlying paper (ex: `9412002v1.pdf`, `9412002v2.pdf`, etc.). We therefore ran `dupremover.py` which kept only the latest version. After this step, the total number of papers in our data set decreased to 20166.

Before we can perform any word counts, however, we had to deal with a typographical issue. Ligatures are linkages between the letters f, l and i in high quality fonts. Since LaTeX uses the computer modern fonts which have ligatures, the document collection was full of them. For example, when I write the word "affluent" it will not be translated into the sequence of characters a,f,f,l,u,e,n,t but instead turn into a,ﬄ,u,e,n,t where ﬄ is a single Unicode character. Can you see the difference between ﬄ and ffl? In order to deal with this issue, I did a preliminary pass using `makewordstream.py` expanding all ligatures to their constituent letters. While I was at it, I also converted all words to lowercase ASCII.

[1]First rule of software development : do not write code – someone has already written it before you.

4.2 Dictionary selection

The next step was to select a subset of all the words that occur in the document collection for which we will perform word counts. A first pass was made on the documents to remove a standard list of stopwords (see `stopwords.py`). Given how large the dataset is we did not feel it was necessary to use word stemming. This way we can capture as much of the granularity of the data as possible.

The total number of unique words of 3 character or more at this step was 67075, and contained lots of non-words like "ijk", which probably refer to matrix indices. While 60k words is not an unreasonable dictionary size, it was deemed too large for our purposes and an effort was made to cut down on the dictionary size. The script `makevocab.py` goes through the word stream and counts total number of occurrences for each word. It then rejects all words that occur less than 45 times in the corpus. We also impose a minimum occurrence threshold of 10000, 6000 and 2000 for three, four and five letter words respectively.

The final pre-processing step selects the top 10011 words by overall frequency and stores it in the file `vocab.txt`. This figure was inspired by the paper [BL09], where they use a vocabulary of this size on a document collection roughly similar to our own.

4.3 Sparse matrix format

The input data that the `topicmodel` program expects is in a standard sparse matrix format which is generated by the script `Makedocword.pl`. The resulting file `docword.txt` contains one row for each unique word in each document. For example, consider the following excerpt:

```
#docword.txt
...
34 376 6
34 6767 5
...
```

These two lines indicate that the document with id=34 contains 6 occurrences of word 376 and 5 occurrences of word 6767. This is the standard bag-of-words paradigm for each document.

The following list summarizes the important details of the finalized data set at the stage when it is read to be fed to the Gibbs sampling inference algorithm.

- Size of vocabulary: $W = 10011$
- Total number of documents: $D = 20166$
- Total number of words in corpus: $N = 41202148$

5 Results

Using the above data set we perfomed a number of runs and recorded the resulting topics and other parameter like runtime and memory usage. We report on our finding in this section.

5.1 Evaluation of extracted topics

The natural application of topic models is the automated extraction of topics from the data set. Given that we have learned the probability family of distributions φ_{tw}, we can now query it to see what are the most common words for each topic. The results of a test run with $T = 20$ topics and $NITER = 300$ iterations of the Gibbs chain are displayed in Table 1 on page 9.

Everytime I ran the algorithm, I was surprized by its amazing power to pick out clusters of words that belong togher. I discussed the words for each topic with some colleagues and they were also amazed at the accuracy of the produced clusters.

5.2 Number of topics

Another factor that needs to be investigated is how the performance of the algorithm varies when different number of topics are sought. We ran a series of experiments with $NITER = 100$ and different values of T randing from 3 to 200.

During the entire test sequence, the memory consumption remained roughtly constant and for all experiments the memory used was roughly 700MB. The running time increased linearly with the number of topics as can be seen from Table 2 below.

5.3 Gibbs sampling chain length

The other parameter we chose to vary in our experiments was the length of the chain which we use for Gibbs sampling. We held the number of topics constant at $T = 20$ and varied the number of iterations from 5 (which would certainly be insufficient) to 300 which is probably overkill.

The running time results are shown in Table 3. The fact that the runtime increases linearly with $NITER$ should come as no surprize since $NITER$ is simply the maximum value of the outermost loop in the Gibbs sampling routine.

The real data which we intended to collect in order to evaluate these runs is the perplexity and not the runtime.

5.4 Perplexity

A quantitative method for evaluating the performance of a topic model is to calculate the perplexity of the document set given the learned parameters.

$$pplex(\mathcal{D}) = \exp\left(-\frac{1}{N} \sum_{1}^{N} \log P(w_n|d_n) \right) = \exp\left(-\frac{1}{N} \sum_{j=1}^{D} \sum_{w=1}^{W} N_{wj} \log P(w|d) \right), \quad (3)$$

The perplexity is a measure of how "surprized" the model is to observe the data $\mathcal{D}$.

I wrote a program `perplexity.py` which computes the perplexity of the data set given the topic-word distribtion φ and the document-topic distribution θ. **Unfortunately**, by the time the moment came to evaluate the data from the various test runs I had been performing during the past days I realized that my script had a major bug in it. The output of each run was overwriting the output of the previous run!

Thus I am forced to give anecdotal calculations of the perplexity based on the last run of each experiment.

- For $NITER = 300$, and $T = 20$ we had $pplex = 1349.88$
- For $NITER = 100$, and $T = 200$ we had $pplex = 952.31$

Aditionally, we did a few short runs with $NITER = 50$ and different number of topics. The results are reported in Table 4.

I must note that the perplexity calculation above may be misleading since it uses the same data for both training and testing. It is conceivable that the model might be overfitting specific patterns in the training set. Thus we can expect to see a decrease in the inbred-test perplexity while at the same time having poor generalization performace. The correct approach would be to separate a portion of the data and use it as a test set according to the detailed procedures outlined in [Hei05].

6 Discussion and Conclusion

This project has been a very good opportunity to learn about LDA and machine learning in general. I learned both theoretical facts about graphical models as well as practical consideraitons about programming inference algorithms, memory management and data pre-processing.

While I was able to extract reasonably good topics from the `quant-ph` archive, I think there is still a lot of interesting experiments to perform with this data set. In particular I would like to use the extracted topics in order to devlop an automated recommendation system or a "topic filter" which would help me keep track of which papers are posted on the arXiv every day that are relevant to my topics of research.

Some other ideas that I would like to pursue are the following.

6.1 Regular expressions counts

In text analysis we invariably use word counts as the main "features" of documents. Since we have the full power and flexibility of python during the pre-processing stage, we could use instead regular expressions as features.

For example we could quantify how many matches to the reg ex "`H(.*)`" there are in each document. Certainly, for papers that deal with information theory this will be a highly informative feature.

Another possible use of regular expressions is to have a digram model with synonyms taken into account. For example we could count how many matches there are to this reglar expression "`quantum (mechanics|physics)`" instead of trying to keep track of the two options separately.

6.2 Two data set correlations

I have not seen in the litterature any discussion about using LDA to automatically create links between two data collections. For example if we trained a topic model on wikipedia articles AND the arXiv, we would be able to automatically generate meaningful links between the two. As you browse the arXiv you could get suggested articles from wikipedia that cover similar topics.

6.3 Parallel LDA

One aspect that I did not get a chance to look into deeper is the use of parallel algorithms for inference of the LDA model. One approach is to modify the Gibbs sampling or variational methods to permit loosely coupled parallel operation [NSS06, NASW07].

Another approach is to use GPU based computation which is highly parallel and vectorized. CUDA (Compute Unified Device Architecture) is a simple API which allows for GPU programming on NVIDIA grpahics boards. The speedups reported are very impressive [MHSO09, YBQ]. This research direciton would also be an excuse for me to buy an expensive graphics card.

6.4 Citation graph

One simple further step that can be taken to make use of the arXiv topic model is to extract the citation graph amongst the paper. This can be done with another regular expression of the form `quant-ph\d{7}` or from some third party source like Citeseer.

Having the citaiton graph would allows us to do a "page rank" type of calculation and extract a sense of importance for the papers in each topic.

I feel this is more of a beginning than an end to this project. I have gotten acquainted with the software and the data set and hopefully I can produce some worthwhile results in the coming months. All the source code and results associated with this project are available here [Sav].

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Table 1: Automatically extracted topics.

Common words in topic	my labelling
(t1) quantum theory mechanics physical classical physics interpretation probability time state space possible principle fact point description properties question sense probabilities ...	general QM
(t2) entanglement states state entangled phys rev pure local lett mixed separable quant systems maximally bipartite measure horodecki concurrence schmidt ghz ...	entanglement
(t3) let theorem set proof follows definition lemma positive case define section defined prove exists consider condition implies holds map finite ...	math jargon
(t4) quantum algorithm problem number probability classical log time computation complexity graph computer algorithms random function polynomial search input problems step ...	computing
(t11) qubit quantum state qubits gate gates control operation computation operations single unitary circuit controlled computer fig universal states implementation sequence ...	computing 2
(t5) state states coherent phys mode rev noise number quantum gaussian modes field squeezing squeezed function vacuum lett phase operator exp ...	optics
(t8) photon photons beam single polarization signal detection fig optical detector interference light rev experimental phys lett experiment source detectors pump ...	optics 2
(t6) measurement quantum measurements state bell probability particle local inequality experiment phys observables observable measured correlations particles probabilities measuring non inequalities ...	Bell inequalities
(t7) space quantum group representation algebra operators operator hilbert invariant theory structure defined lie dimensional classical functions product vector form representations ...	algebra
(t9) spin hamiltonian phys energy state model rev interaction ground magnetic states coupling spins lett systems quantum lattice electron field interactions ...	physics
(t15) atom field atoms cavity atomic state frequency laser rev level phys transition coupling resonance interaction pulse trap fig optical ion ...	atomic phys
(t16) equation function potential phys solution functions equations energy solutions form order hamiltonian exp integral schrdinger problem case real oscillator terms ...	schrodinger
(t18) time quantum evolution initial classical dynamics decoherence equation environment systems phys hamiltonian density stochastic process decay dynamical model interaction state ...	decoherence
(t10) error quantum code errors codes correction noise qubits encoded encoding block number level stabilizer fault probability rate pauli threshold measurement ...	error correction
(t12) wave particle field energy momentum particles time force mass function phys scattering motion free relativistic position theory velocity fields effect ...	field theory
(t13) phase cos sin exp case function phys momentum distribution angle initial obtain wigner geometric classical phases angular axis consider rotation ...	particle physics
(t14) fig results values line figure large small case numerical number shown parameters order parameter region obtained function shows limit average ...	science jargon
(t17) matrix operator operators states basis density matrices form vector unitary elements state set vectors product case diagonal eigenvalues terms orthogonal ...	linear algebra
(t19) alice bob quantum protocol key communication information classical state bit teleportation scheme eve protocols bits basis security bobs channel alices ...	crypto
(t20) information quantum state states entropy optimal channel fidelity probability log measurement classical input channels pure output cloning ensemble capacity povm ...	information theory

Table 2: Runtime as a function of number of topics.

T	runtime (s)
3	1447
5	1650
10	2079
15	2538
20	2857
25	3248
30	3601
40	4230
50	4924
75	6610
100	8130
150	11183
200	14167

Table 3: Runtime as a function of length of Gibbs sampling.

NITER	runtime (s)
5	229
10	407
20	768
30	1138
50	1861
75	2772
100	3742
150	5535
200	7424
300	10993

Table 4: Perplexity as a function of T. $NITER = 50$

T	perplexity
5	1652.76
10	1486.31
15	1417.64
20	1361.29
30	1296.80