Parameter estimation for text analysis

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Abstract. Presents parameter estimation methods common with discrete probability distributions, which is of particular interest in text modeling. Starting with maximum likelihood, a posteriori and Bayesian estimation, central concepts like conjugate distributions and Bayesian networks are reviewed. As an application, the model of latent Dirichlet allocation (LDA) is explained in detail with a full derivation of an approximate inference algorithm based on Gibbs sampling, including a discussion of Dirichlet hyperparameter estimation. Finally, analysis methods of LDA models are discussed.

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1 Introduction

This technical report is intended to review the foundations of parameter estimation in the discrete domain, which is necessary to understand the inner workings of topic-based text analysis approaches like probabilistic latent semantic analysis (PLSA) [Hofm99], latent Dirichlet allocation (LDA) [BNJ02] and other mixture models of count data. Despite their general acceptance in the research community, it appears that there is no common book or introductory paper that fills this role: Most known texts use examples from the Gaussian domain, where formulations appear to be rather different. Other very good introductory work on topic models (e.g., [StGr07]) skips details of algorithms and other background for clarity of presentation.

We therefore will systematically introduce the basic concepts of parameter estimation with a couple of simple examples on binary data in Section 2. We then will introduce the concept of conjugacy along with a review of the most common probability distributions needed in the text domain in Section 3. The joint presentation of conjugacy with associated real-world conjugate pairs directly justifies the choice of distributions introduced. Section 4 will introduce Bayesian networks as a graphical language to describe systems via their probabilistic models.

With these basic concepts, we present the idea of latent Dirichlet allocation (LDA) in Section 5, a flexible model to estimate the properties of text. On the example of LDA, the usage of Gibbs sampling is shown as a straight-forward means of approximate inference in Bayesian networks. Two other important aspects of LDA are discussed afterwards: In Section 6, the influence of LDA hyperparameters is discussed and an estimation method proposed, and in Section 7, methods are presented to analyse LDA models for querying and evaluation.

2 Parameter estimation approaches

We face two inference problems, (1) to estimate values for a set of distribution parameters ϑ that can best explain a set of observations $\mathcal{X}$ and (2) to calculate the probability of new observations $\tilde{x}$ given previous observations, i.e., to find $p(\tilde{x}|\mathcal{X})$. We will refer to the former problem as the estimation problem and to the latter as the prediction or regression problem.

The data set $\mathcal{X} \triangleq \{x_i\}_{i=1}^{|\mathcal{X}|}$ can be considered a sequence of independent and identically distributed (i.i.d.) realisations of a random variable (r.v.) X. The parameters ϑ are dependent on the distributions considered, e.g., for a Gaussian, $\vartheta = \{\mu, \sigma^2\}$.

For these data and parameters, a couple of probability functions are ubiquitous in Bayesian statistics. They are best introduced as parts of Bayes' rule, which is[1]:

$$\text{argmax\_theta}\, p(\vartheta|\mathcal{X}) = \frac{p(\mathcal{X}|\vartheta) \cdot p(\vartheta)}{p(\mathcal{X})}, \tag{1}$$

and we define the corresponding terminology:

$$\text{posterior} = \frac{\text{likelihood} \cdot \text{prior}}{\text{evidence}}. \tag{2}$$

In the next paragraphs, we will show different estimation methods that start from simple maximisation of the likelihood, then show how prior belief on parameters can be incorporated by maximising the posterior and finally use Bayes' rule to infer a complete posterior distribution.

2.1 Maximum likelihood estimation

Maximum likelihood (ML) estimation tries to find parameters that maximise the likelihood,[2]

$$L(\vartheta|\mathcal{X}) \triangleq p(\mathcal{X}|\vartheta) = \bigcap_{x \in \mathcal{X}} \{X = x|\vartheta\} = \prod_{x \in \mathcal{X}} p(x|\vartheta), \tag{3}$$

i.e., the probability of the joint event that X generates the data $\mathcal{X}$. Because of the product in Eq. 3, it is often simpler to use the log likelihood, $\mathcal{L} \triangleq \log L$. The ML estimation problem then can be written as:

$$\hat{\vartheta}_{\text{ML}} = \underset{\vartheta}{\text{argmax}}\, \mathcal{L}(\vartheta|\mathcal{X}) = \underset{\vartheta}{\text{argmax}} \sum_{x \in \mathcal{X}} \log p(x|\vartheta). \tag{4}$$

The common way to obtain the parameter estimates is to solve the system:

$$\frac{\partial \mathcal{L}(\vartheta|\mathcal{X})}{\partial \vartheta_k} \stackrel{!}{=} 0 \quad \forall \vartheta_k \in \vartheta. \tag{5}$$

[1] Derivation: $p(\vartheta|\mathcal{X}) \cdot p(\mathcal{X}) = p(\mathcal{X}, \vartheta) = p(\mathcal{X}|\vartheta) \cdot p(\vartheta)$.

[2] Note that here $p(\mathcal{X}|\vartheta)$ is a function of the condition ϑ with $\mathcal{X}$ fixed.

The probability of a new observation $\tilde{x}$ given the data $\mathcal{X}$ can now be found using the approximation[3]:

$$p(\tilde{x}|\mathcal{X}) = \int_{\vartheta\in\Theta} p(\tilde{x}|\vartheta)\, p(\vartheta|\mathcal{X})\, \mathrm{d}\vartheta \tag{6}$$

$$\approx \int_{\vartheta\in\Theta} p(\tilde{x}|\hat{\vartheta}_{\mathrm{ML}})\, p(\vartheta|\mathcal{X})\, \mathrm{d}\vartheta = p(\tilde{x}|\hat{\vartheta}_{\mathrm{ML}}), \tag{7}$$

that is, the next sample is anticipated to be distributed with the estimated parameters $\hat{\vartheta}_{\mathrm{ML}}$.

As an example, consider a set C of N Bernoulli experiments with unknown parameter p, e.g., realised by tossing a deformed coin. The Bernoulli density function for the r.v. C for one experiment is:

$$p(C{=}c|p) = p^c\,(1-p)^{1-c} \triangleq \mathrm{Bern}(c|p) \tag{8}$$

p(C=heads)=p
p(C=tails)=(1-p)

where we define c=1 for heads and c=0 for tails[4].

Building an ML estimator for the parameter p can be done by expressing the (log) likelihood as a function of the data:

$$\mathcal{L} = \log \prod_{i=1}^{N} p(C{=}c_i|p) = \sum_{i=1}^{N} \log p(C{=}c_i|p) \tag{9}$$

$$= n^{(1)} \log p(C{=}1|p) + n^{(0)} \log p(C{=}0|p)$$

$$= n^{(1)} \log p + n^{(0)} \log(1-p) \tag{10}$$

where $n^{(c)}$ is the number of times a Bernoulli experiment yielded event c. Differentiating with respect to (w.r.t.) the parameter p yields:

$$\frac{\partial \mathcal{L}}{\partial p} = \frac{n^{(1)}}{p} - \frac{n^{(0)}}{1-p} \stackrel{!}{=} 0 \quad \Leftrightarrow \quad \hat{p}_{\mathrm{ML}} = \frac{n^{(1)}}{n^{(1)}+n^{(0)}} = \frac{n^{(1)}}{N}, \tag{11}$$

which is simply the ratio of heads results to the total number of samples. To put some numbers into the example, we could imagine that our coin is strongly deformed, and after 20 trials, we have $n^{(1)}$=12 times heads and $n^{(0)}$=8 times tails. This results in an ML estimation of of $\hat{p}_{\mathrm{ML}} = 12/20 = 0.6$.

2.2 Maximum a posteriori estimation

Maximum a posteriori (MAP) estimation is very similar to ML estimation but allows to include some a priori belief on the parameters by weighting them with a prior distribution $p(\vartheta)$. The name derives from the objective to maximise the posterior of the parameters given the data:

$$\hat{\vartheta}_{\mathrm{MAP}} = \operatorname*{argmax}_{\vartheta}\, p(\vartheta|\mathcal{X}). \tag{12}$$

[3] The ML estimate $\hat{\vartheta}_{\mathrm{ML}}$ is considered a constant, and the integral over the parameters given the data is the total probability that integrates to one.

[4] The notation in Eq. 8 is somewhat peculiar because it makes use of the values of c to "filter" the respective parts in the density function and additionally uses these numbers to represent disjoint events.

By using Bayes' rule (Eq. 1), this can be rewritten to:

$$\begin{aligned}\hat{\vartheta}_{\text{MAP}} &= \underset{\vartheta}{\text{argmax}}\ \frac{p(\mathcal{X}|\vartheta)p(\vartheta)}{p(\mathcal{X})} \qquad \Big| \ p(\mathcal{X}) \neq f(\vartheta) \\ &= \underset{\vartheta}{\text{argmax}}\ p(\mathcal{X}|\vartheta)p(\vartheta) = \underset{\vartheta}{\text{argmax}}\ \{\mathcal{L}(\vartheta|\mathcal{X}) + \log p(\vartheta)\} \\ &= \underset{\vartheta}{\text{argmax}}\ \Big\{\sum_{x\in\mathcal{X}} \log p(x|\vartheta)\ +\ \log p(\vartheta)\Big\}. \end{aligned} \tag{13}$$

Since the max is achieved for the same theta

Compared to Eq. 4, a prior distribution is added to the likelihood. In practice, the prior $p(\vartheta)$ can be used to encode extra knowledge as well as to prevent overfitting by enforcing preference to simpler models, which is also called Occam's razor[5].

With the incorporation of $p(\vartheta)$, MAP follows the Bayesian approach to data modelling where the parameters ϑ are thought of as r.v.s. With priors that are parametrised themselves, i.e., $p(\vartheta) := p(\vartheta|\alpha)$ with hyperparameters α, the belief in the anticipated values of ϑ can be expressed within the framework of probability[6], and a hierarchy of parameters is created.

MAP parameter estimates can be found by maximising the term $\mathcal{L}(\vartheta|\mathcal{X}) + \log p(\vartheta)$, similar to Eq. 5. Analogous to Eq. 7, the probability of a new observation, $\tilde{x}$, given the data, $\mathcal{X}$, can be approximated using:

$$p(\tilde{x}|\mathcal{X}) \approx \int_{\vartheta\in\Theta} p(\tilde{x}|\hat{\vartheta}_{\text{MAP}})\, p(\vartheta|\mathcal{X})\, \mathrm{d}\vartheta = p(\tilde{x}|\hat{\vartheta}_{\text{MAP}}). \tag{14}$$

Returning to the simplistic demonstration on ML, we can give an example for the MAP estimator. Consider the above experiment, but now there are values for p that we believe to be more likely, e.g., we believe that a coin usually is fair. This can be expressed as a prior distribution that has a high probability around 0.5. We choose the beta distribution:

$$p(p|\alpha,\beta) = \frac{1}{\mathrm{B}(\alpha,\beta)} p^{\alpha-1}(1-p)^{\beta-1} \triangleq \text{Beta}(p|\alpha,\beta), \tag{15}$$

with the beta function $\mathrm{B}(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$. The function $\Gamma(x)$ is the Gamma function, which can be understood as a generalisation of the factorial to the domain of real numbers via the identity $x! = \Gamma(x+1)$. The beta distribution supports the interval [0,1] and therefore is useful to generate normalised probability values. For a graphical representation of the beta probability density function (pdf), see Fig. 1. As can be seen, with different parameters the distribution takes on quite different pdfs.

In our example, we believe in a fair coin and set $\alpha = \beta = 5$, which results in a distribution with a mode (maximum) at 0.5. The optimisation problem now becomes

[5] Pluralitas non est ponenda sine necessitate = Plurality should not be posited without necessity. Occam's razor is also called the principle of parsimony.

[6] Belief is not identical to probability, which is one of the reasons why Bayesian approaches are disputed by some theorists despite their practical importance.

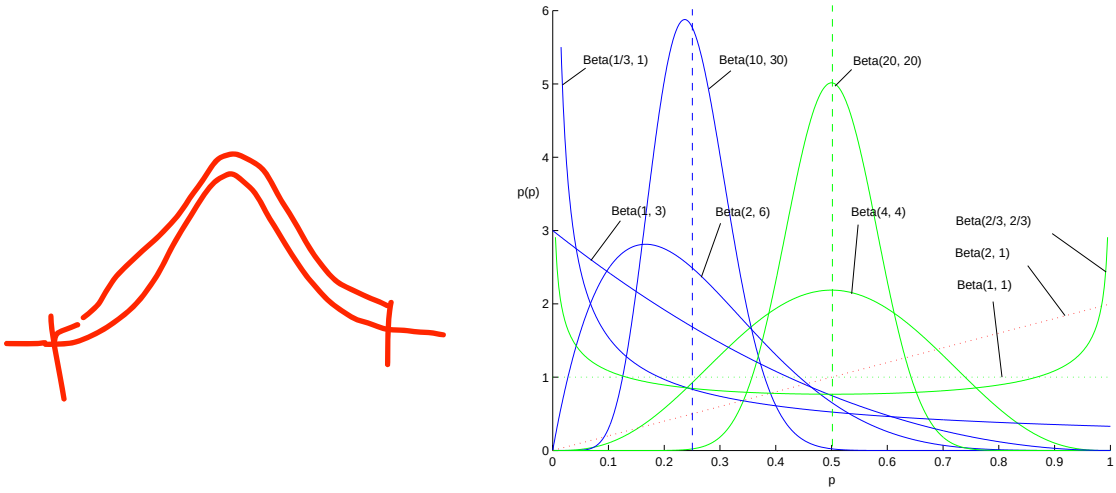

Fig. 1. Density functions of the beta distribution with different symmetric and asymmetric parametrisations.

(cf. Eq. 11):

$$\frac{\partial}{\partial p}\mathcal{L} + \log p(p) = \frac{n^{(1)}}{p} - \frac{n^{(0)}}{1-p} + \frac{\alpha-1}{p} - \frac{\beta-1}{1-p} \stackrel{!}{=} 0 \tag{16}$$

$$\Leftrightarrow \quad \hat{p}_{\mathrm{MAP}} = \frac{n^{(1)}+\alpha-1}{n^{(1)}+n^{(0)}+\alpha+\beta-2} = \frac{n^{(1)}+4}{n^{(1)}+n^{(0)}+8} \tag{17}$$

This result is interesting in two aspects. The first one is the changed behaviour of the estimate $\hat{p}_{\mathrm{MAP}}$ w.r.t. the counts $n^{(c)}$: their influence on the estimate is reduced by the additive values that "pull" the value towards $\hat{p}_{\mathrm{MAP}} = 4/8 = 0.5$. The higher the values of the hyperparameters α and β, the more actual observations are necessary to revise the belief expressed by them. The second interesting aspect is the exclusive appearance of the sums $n^{(1)}+\alpha-1$ and $n^{(0)}+\beta-1$: It is irrelevant whether the counts actually derive from actual observations or prior belief expressed as hypervariables. This is why the hyperparameters α and β are often referred to as pseudo-counts. The higher pseudo-counts exist, the sharper the beta distribution is concentrated around its maximum. Again, we observe in 20 trials $n^{(1)}$=12 times heads and $n^{(0)}$=8 times tails. This results in an MAP estimation of $\hat{p}_{\mathrm{MAP}} = 16/28 = 0.571$, which in comparison to $\hat{p}_{\mathrm{ML}} = 0.6$ shows the influence of the prior belief of the "fairness" of the coin.

2.3 Bayesian inference

Bayesian inference extends the MAP approach by allowing a distribution over the parameter set ϑ instead of making a direct estimate. Not only encodes this the maximum

(a posteriori) value of the data-generated parameters, but it also incorporates expectation as another parameter estimate as well as variance information as a measure of estimation quality or confidence. The main step in this approach is the calculation of the posterior according to Bayes' rule:

$$p(\vartheta|\mathcal{X}) = \frac{p(\mathcal{X}|\vartheta) \cdot p(\vartheta)}{p(\mathcal{X})}. \tag{18}$$

As we do not restrict the calculation to finding a maximum, it is necessary to calculate the normalisation term, i.e., the probability of the "evidence", $p(\mathcal{X})$, in Eq. 18. Its value can be expressed by the total probability w.r.t. the parameters[7]:

$$p(\mathcal{X}) = \int_{\vartheta \in \Theta} p(\mathcal{X}|\vartheta)\, p(\vartheta)\, \mathrm{d}\vartheta. \tag{19}$$

As new data are observed, the posterior in Eq. 18 is automatically adjusted and can eventually be analysed for its statistics. However, often the normalisation integral in Eq. 19 is the intricate part of Bayesian inference, which will be treated further below.

In the prediction problem, the Bayesian approach extends MAP by ensuring an exact equality in Eq. 14, which then becomes:

$$p(\tilde{x}|\mathcal{X}) = \int_{\vartheta \in \Theta} p(\tilde{x}|\vartheta)\, p(\vartheta|\mathcal{X})\, \mathrm{d}\vartheta \tag{20}$$

$$= \int_{\vartheta \in \Theta} p(\tilde{x}|\vartheta)\, \frac{p(\mathcal{X}|\vartheta)p(\vartheta)}{p(\mathcal{X})}\, \mathrm{d}\vartheta \tag{21}$$

Here the posterior $p(\vartheta|\mathcal{X})$ replaces an explicit calculation of parameter values ϑ. By integration over ϑ, the prior belief is automatically incorporated into the prediction, which itself is a distribution over $\tilde{x}$ and can again be analysed w.r.t. confidence, e.g., via its variance.

As an example, we build a Bayesian estimator for the above situation of having N Bernoulli observations and a prior belief that is expressed by a beta distribution with parameters $(5, 5)$, as in the MAP example. In addition to the maximum a posteriori value, we want the expected value of the now-random parameter p and a measure of estimation confidence. Including the prior belief, we obtain[8]:

$$p(p|C, \alpha, \beta) = \frac{\prod_{i=1}^{N} p(C{=}c_i|p)\; p(p|\alpha,\beta)}{\int_0^1 \prod_{i=1}^{N} p(C{=}c_i|p)\; p(p|\alpha,\beta)\, \mathrm{d}p} \tag{22}$$

$$= \frac{p^{n^{(1)}}(1-p)^{n^{(0)}}\, \frac{1}{\mathrm{B}(\alpha,\beta)} p^{\alpha-1}(1-p)^{\beta-1}}{Z} \tag{23}$$

$$= \frac{p^{[n^{(1)}+\alpha]-1}(1-p)^{[n^{(0)}+\beta]-1}}{\mathrm{B}(n^{(1)}+\alpha, n^{(0)}+\beta)} \tag{24}$$

$$= \mathrm{Beta}(p|n^{(1)}+\alpha, n^{(0)}+\beta) \tag{25}$$

[7] This marginalisation is why evidence is also refered to as "marginal likelihood". The integral is used here as a generalisation for continuous and discrete sample spaces, where the latter require sums.

[8] The marginal likelihood Z in the denominator is simply determined by the normalisation constraint of the beta distribution.

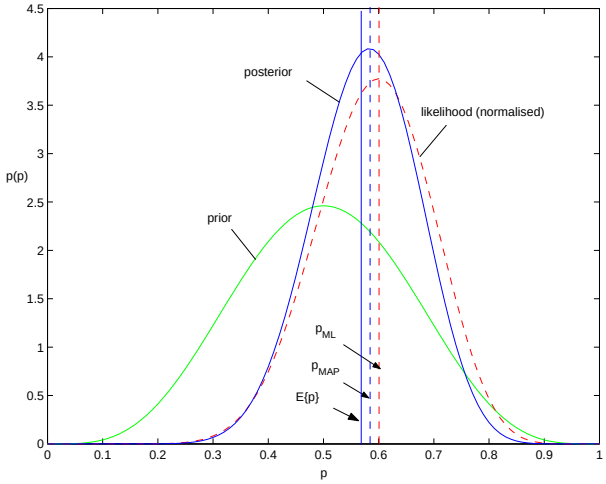

Fig. 2. Visualising the coin experiment.

The Beta(α,β) distribution has mean, $\langle p|\alpha,\beta\rangle = \alpha(\alpha+\beta)^{-1}$, and variance, $\mathsf{V}\{p|\alpha,\beta\} = \alpha\beta(\alpha+\beta+1)^{-1}(\alpha+\beta)^{-2}$. Using these statistics, our estimation result is:

$$\langle p|C\rangle = \frac{n^{(1)}+\alpha}{n^{(1)}+n^{(0)}+\alpha+\beta} = \frac{n^{(1)}+5}{N+10} \tag{26}$$

$$\mathsf{V}\{p|C\} = \frac{(n^{(1)}+\alpha)(n^{(0)}+\beta)}{(N+\alpha+\beta+1)(N+\alpha+\beta)^2} = \frac{(n^{(1)}+5)(n^{(0)}+5)}{(N+11)(N+10)^2} \tag{27}$$

The expectation is not identical to the MAP estimate (see Eq. 17), which literally is the maximum and not the expected value of the posterior. However, if the sums of the counts and pseudo-counts become larger, both expectation and maximum converge. With the 20 coin observations from the above example ($n^{(1)}$=12 and $n^{(0)}$=8), we obtain the situation depicted in Fig. 2. The Bayesian estimation values are $\langle p|C\rangle = 17/30 = 0.567$ and $\mathsf{V}\{p|C\} = 17\cdot 13/(31\cdot 30^2) = 0.0079$.

3 Conjugate distributions

Calculation of Bayesian models often becomes quite difficult, e.g., because the summations or integrals of the marginal likelihood are intractable or there are unknown variables. Fortunately, the Bayesian approach leaves some freedom to the encoding of prior belief, and a frequent strategy to facilitate model inference is to use *conjugate prior* distributions.

3.1 Conjugacy

A conjugate prior, $p(\vartheta)$, of a likelihood, $p(x|\vartheta)$, is a distribution that results in a posterior distribution, $p(\vartheta|x)$ with the same functional form as the prior and a parameterisation

that incorporates the observations x. The last example (Eq. 25 and above) illustrates this: The posterior turned out to be a beta distribution like the prior with parameters that incorporated the count statistics of observations. Notably, the crucial determination of the normalising term $1/Z$ turned out to be simple.

In addition to calculational simplifications, conjugacy often results in meaningful interpretations of hyperparameters, and in our beta–Bernoulli case, the resulting posterior can be interpreted as the prior with the observation counts $n^{(c)}$ added to the pseudo-counts α and β (see Eq. 25).

Moreover, conjugate prior-likelihood pairs often allow to marginalise out the likelihood parameters in closed form and thus express the likelihood of observations directly in terms of hyperparameters. For the beta–Bernoulli case, this looks as follows[9]:

$$p(C|\alpha,\beta) = \int_0^1 p(C|p)\; p(p|\alpha,\beta)\,\mathrm{d}p \tag{28}$$

$$= \int_0^1 p^{n^{(1)}}(1-p)^{n^{(0)}}\;\frac{1}{\mathrm{B}(\alpha,\beta)}p^{\alpha-1}(1-p)^{\beta-1}\,\mathrm{d}p \tag{29}$$

$$= \frac{1}{\mathrm{B}(\alpha,\beta)}\int_0^1 p^{n^{(1)}+\alpha-1}(1-p)^{n^{(0)}+\beta-1}\,\mathrm{d}p \qquad \Big|\ \text{Beta}\int \tag{30}$$

$$= \frac{\mathrm{B}(n^{(1)}+\alpha, n^{(0)}+\beta)}{\mathrm{B}(\alpha,\beta)} = \frac{\Gamma(n^{(1)}+\alpha)\Gamma(n^{(0)}+\beta)}{\Gamma(n^{(1)}+n^{(0)}+\alpha+\beta)}\,\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}. \tag{31}$$

This result can be used to make predictions on the distribution of future Bernoulli trials without explicit knowledge of the parameter p but from prior observations. This is expressed with the predictive likelihood for a new observation[10]:

$$p(\tilde{c}{=}1|C,\alpha,\beta) = \frac{p(\tilde{c}{=}1,C|\alpha,\beta)}{p(C|\alpha,\beta)} = \frac{\frac{\Gamma(n^{(1)}+1+\alpha)}{\Gamma(n^{(1)}+1+n^{(0)}+\alpha+\beta)}}{\frac{\Gamma(n^{(1)}+\alpha)}{\Gamma(n^{(1)}+n^{(0)}+\alpha+\beta}} \tag{32}$$

$$= \frac{n^{(1)}+\alpha}{n^{(1)}+n^{(0)}+\alpha+\beta}. \tag{33}$$

There are a couple of important prior–likelihood pairs that can be used to simplify Bayesian inference as described above. One important example related to the beta distribution is the binomial distribution, which gives the probability that exactly $n^{(1)}$ heads from the N Bernoulli experiments with parameter p are observed:

$$p(n^{(1)}|p,N) = \binom{N}{n^{(1)}}p^{n^{(1)}}(1-p)^{n^{(0)}} \triangleq \mathrm{Bin}(n^{(1)}|p,N) \tag{34}$$

As the parameter p has the same meaning as with the Bernoulli distribution, it comes not as a surprise that the conjugate prior on the parameter p of a binomial distribution is a beta distribution, as well. Other distributions that count Bernoulli trials also fall into this scheme, such as the negative-binomial distribution.

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[9] In the calculation, the identity of the beta integral, $\int_0^1 x^a(1-x)^b\,\mathrm{d}x = \mathrm{B}(a+1,b+1)$ is used, also called Eulerian integral of the first kind.

[10] Here the identity $\Gamma(x+1) = x\Gamma(x)$ is used.

3.2 Multivariate case

The distributions considered so far handle outcomes of binary experiments. If we generalise the number of possible events from 2 to a finite integer K, we can obtain a K-dimensional Bernoulli or *multinomial* experiment, e.g., the roll of a die. If we repeat this experiment, we obtain a multinomial distribution of the counts of the observed events (faces of the die), which generalises the binomial distribution:

$$p(\vec{n}|\vec{p}, N) = \binom{N}{\vec{n}} \prod_{k=1}^{K} p_k^{n^{(k)}} \triangleq \text{Mult}(\vec{n}|\vec{p}, N) \tag{35}$$

with the multinomial coefficient $\binom{N}{\vec{n}} = \frac{N!}{\prod_k n^{(k)}!}$. Further, the elements of $\vec{p}$ and $\vec{n}$ follow the constraints $\sum_k p_k = 1$ and $\sum_k n^{(k)} = N$ (cf. the terms $(1-p)$ and $n^{(1)} + n^{(0)} = N$ in the binary case).

The multinomial distribution governs the multivariate variable $\vec{n}$ with elements $n^{(k)}$ that count the occurrences of event k within N total trials, and the multinomial coefficient counts the number of configurations of individual trials that lead to the total.

A single multinomial trial generalises the Bernoulli distribution to a discrete categorical distribution:

$$p(\vec{n}|\vec{p}) = \prod_{k=1}^{K} p_k^{n^{(k)}} = \text{Mult}(\vec{n}|\vec{p}, 1) \tag{36}$$

where the count vector $\vec{n}$ is zero except for a single element $n^{(z)}$=1. Hence we can simplify the product and replace the multivariate count vector by the index of the nonzero element z as an alternative notation:

$$p(z|\vec{p}) = p_z \triangleq \text{Mult}(z|\vec{p}), \tag{37}$$

which is identical to the general discrete distribution $\text{Disc}(\vec{p})$. Introducing the multinomial r.v. C, the likelihood of N repetitions of a multinomial experiment (cf. Eq. 9), the obervation set C, becomes:

$$p(C|\vec{p}) = \prod_{n=1}^{N} \text{Mult}(C{=}z_i|\vec{p}) = \prod_{n=1}^{N} p_{z_i} = \prod_{k=1}^{K} p_k^{n^{(k)}}, \tag{38}$$

which is just the multinomial distribution with a missing normalising multinomial coefficient. This difference is due to the fact that we assume a sequence of outcomes of the N experiments instead of getting the probability of a particular multinomial count vector $\vec{n}$, which could be generated by $\binom{N}{\vec{n}}$ different sequences C.[11] In modelling text observations, this last form of a repeated multinomial experiment is quite important. For the parameters $\vec{p}$ of the multinomial distribution, the conjugate prior is the Dirichlet

[11] In a binary setting, this corresponds to the difference between the observations from a repeated Bernoulli trial and the probability of (any) $n^{(1)}$ successes, which is described by the binomial distribution.

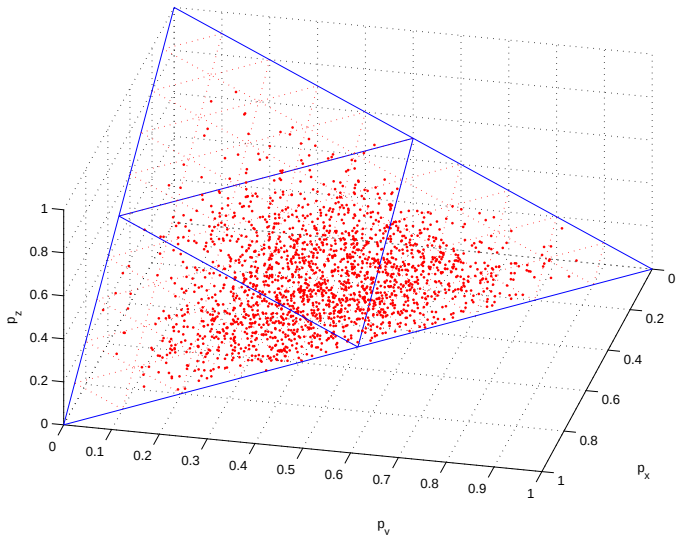

Fig. 3. 2000 samples from a Dirichlet distribution Dir(4, 4, 2). The plot shows that all samples are on a simplex embedded in the three-dimensional space, due to the constraint $\sum_k p_k = 1$.

distribution, which generalises the beta distribution from 2 to K dimensions:

$$p(\vec{p}|\vec{\alpha}) = \mathrm{Dir}(\vec{p}|\vec{\alpha}) \triangleq \frac{\Gamma(\sum_{k=1}^{K} \alpha_k)}{\prod_{k=1}^{K} \Gamma(\alpha_k)} \prod_{k=1}^{K} p_k^{\alpha_k - 1} \tag{39}$$

$$\triangleq \frac{1}{\Delta(\vec{\alpha})} \prod_{k=1}^{K} p_k^{\alpha_k - 1}, \quad \Delta(\vec{\alpha}) = \frac{\prod_{k=1}^{\dim \vec{\alpha}} \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^{\dim \vec{\alpha}} \alpha_k)}, \tag{40}$$

with parameters $\vec{\alpha}$ and the "Dirichlet delta function" $\Delta(\vec{\alpha})$, which we introduce for notational convenience[12]. An example of a Dirichlet distribution can be seen in Fig. 3. In many applications, a symmetric Dirichlet distribution is used, which is defined in terms of a scalar parameter $\alpha = \sum \alpha_k / K$ and the dimension K:

$$p(\vec{p}|\alpha, K) = \mathrm{Dir}(\vec{p}|\alpha, K) \triangleq \frac{\Gamma(K\alpha)}{\Gamma(\alpha)^K} \prod_{k=1}^{K} p_k^{\alpha - 1} \tag{41}$$

$$\triangleq \frac{1}{\Delta_K(\alpha)} \prod_{k=1}^{K} p_k^{\alpha - 1}, \quad \Delta_K(\alpha) = \frac{\Gamma(\alpha)^K}{\Gamma(K\alpha)}. \tag{42}$$

[12] The function $\Delta(\vec{\alpha})$ can be seen as a multidimensional extension to the beta function: $\mathrm{B}(\alpha_1, \alpha_2) = \Delta(\{\alpha_1, \alpha_2\})$. It comes as a surprise that this notation is not used in the literature, especially since $\Delta(\vec{\alpha})$ can be shown to be the Dirichlet integral of the first kind for the summation function $f(\Sigma x_i)$=1: $\Delta(\vec{\alpha}) = \int_{\Sigma x_i = 1} \prod_i^N x_i^{\alpha_i - 1} \, \mathrm{d}^N \vec{x}$, analogous to the beta integral: $\mathrm{B}(\alpha_1, \alpha_2) = \int_0^1 x^{\alpha_1 - 1}(1 - x)^{\alpha_2 - 1} \, \mathrm{d}x$.

3.3 Modelling text

Consider a set $\mathcal{W}$ of N i.i.d. draws from a multinomial random variable W. This can be imagined as drawing N words w from a vocabulary $\mathcal{V}$ of size V. The likelihood of these samples is simply:

$$L(\vec{p}|\vec{w}) = p(\mathcal{W}|\vec{p}) = \prod_{t=1}^{V} p_t^{n^{(t)}}, \quad \sum_{t=1}^{V} n^{(t)} = N, \quad \sum_{t=1}^{V} p_t = 1, \tag{43}$$

where $n^{(t)}$ is the number of times term t was observed as a word[13]. This example is the unigram model, which assumes a general distribution of terms of a vocabulary $\mathcal{V}$, $\text{Mult}(t \in \mathcal{V}|\vec{p})$, where $\vec{p}$ is the probability that term t is observed as word w in a document. The unigram model assumes just one likelihood for the entire text considered, which is for instance useful for general assumptions about a language or corpus but does not differentiate between any partial sets, e.g., documents. In addition, it is a perfect basis to develop more complex models.

Assuming conjugacy, the parameter vector $\vec{p}$ of the vocabulary can be modelled with a Dirichlet distribution, $\vec{p} \sim \text{Dir}(\vec{p}|\vec{\alpha})$. Analogous to Eq. 25, we obtain the important property of the Dirichlet posterior to merge multinomial observations $\mathcal{W}$ with prior pseudo-counts $\vec{\alpha}$:

$$p(\vec{p}|\mathcal{W}, \vec{\alpha}) = \frac{\prod_{n=1}^{N} p(w_n|\vec{p})\ p(\vec{p}|\vec{\alpha})}{\int_{\mathcal{P}} \prod_{n=1}^{N} p(w_n|\vec{p})\ p(\vec{p}|\vec{\alpha})\, \mathrm{d}\vec{p}} \tag{44}$$

$$= \frac{1}{Z} \prod_{t=1}^{V} p^{n^{(t)}}\ \frac{1}{\Delta(\vec{\alpha})} p^{\alpha_t - 1} \tag{45}$$

$$= \frac{1}{\Delta(\vec{\alpha} + \vec{n})} \prod_{t=1}^{V} p^{\alpha_t + n^{(t)} - 1} \tag{46}$$

$$= \text{Dir}(\vec{p}|\vec{\alpha} + \vec{n}). \tag{47}$$

Here the likelihood of the words $\prod_{n=1}^{N} p(w_n|\vec{p})$ was rewritten to that of repeated terms $\prod_{t=1}^{V} p(w{=}t|\vec{p})^{n^{(t)}}$ and the known normalisation of the Dirichlet distribution used. The pseudo-count behaviour of the Dirichlet corresponds to the important Pólya urn scheme: An urn contains W balls of V colours, and for each sample of a ball $\tilde{w}$, the ball is replaced and an additional ball of the same colour added (sampling with over-replacement). That is, the Dirichlet exhibits a "rich get richer" or clustering behaviour.

It is often useful to model a new text in terms of the term counts from prior observations instead of some unigram statistics, $\vec{p}$. This can be done using the Dirichlet pseudo-counts hyperparameter and marginalising out the multinomial parameters $\vec{p}$:

$$p(\mathcal{W}|\vec{\alpha}) = \int_{\vec{p} \in \mathcal{P}} p(\mathcal{W}|\vec{p})\ p(\vec{p}|\vec{\alpha})\, \mathrm{d}^V \vec{p} \tag{48}$$

[13] Term refers to the element of a vocabulary, and word refers to the element of a document, respectively. We refer to terms if the category in a multinomial is meant and to words if a particular observation or count is meant. Thus a term can be instantiated by several words in a text corpus.

Compared to the binary case in Eq. 30, the integration limits are not [0,1] any more, as the formulation of the multinomial distribution does not explicitly include the probability normalisation constraint $\sum_k p_k{=}1$. With this constraint added, the integration domain $\mathcal{P}$ becomes a plane $(K-1)$-simplex embedded in the K-dimensional space that is bounded by the lines connecting points $p_k{=}1$ on the axis of each dimension k – see Fig. 3 for three dimensions.[14]

$$p(\mathcal{W}|\vec{\alpha}) = \int_{\vec{p}\in\mathcal{P}} \prod_{n=1}^{N} \mathrm{Mult}(W{=}w_n|\vec{p},1)\ \mathrm{Dir}(\vec{p}|\vec{\alpha})\,\mathrm{d}\vec{p} \tag{49}$$

$$= \int_{\vec{p}\in\mathcal{P}} \prod_{v=1}^{V} p_v^{n^{(v)}} \frac{1}{\Delta(\vec{\alpha})} \prod_{v=1}^{V} p_v^{\alpha_v-1}\,\mathrm{d}^V\vec{p} \tag{50}$$

$$= \frac{1}{\Delta(\vec{\alpha})} \int_{\vec{p}\in\mathcal{P}} \prod_{v=1}^{V} p_v^{n^{(v)}+\alpha_v-1}\,\mathrm{d}^V\vec{p} \qquad \Big|\ \text{Dirichlet}\int \tag{51}$$

$$= \frac{\Delta(\vec{n}+\vec{\alpha})}{\Delta(\vec{\alpha})}, \quad \vec{n} = \{n^{(v)}\}_{v=1}^{V} \tag{52}$$

Similar to the beta–Bernoulli case, the result states a distribution over terms observed as words given a pseudo-count of terms already observed, without any other statistics. More importantly, a similar marginalisation of a parameter is central for the formulation of posterior inference in LDA further below. The distribution in Eq. 52 has also been called the Dirichlet–multinomial distribution or Pólya distribution.

4 Bayesian networks and generative processes

This section reviews two closely connected methodologies to express probabilistic behaviour of a system or phenomenon: Bayesian networks, where conditional statistical independence is an important aspect, and generative processes that can be used to intuitively express observations in terms of random distributions.

4.1 Bayesian networks

Bayesian networks (BNs) are a formal graphical language to express the joint distribution of a system or phenomenon in terms of random variables and their conditional dependencies in a directed graph. BNs are a special case of Graphical Models, an important methodology in machine learning [Murp01] that includes also undirected graphical

[14] In the calculation, we use the Dirichlet integral of the first kind (over simplex $\mathcal{T}$):

$$\int_{\vec{t}\in\mathcal{T}} f(\textstyle\sum_i^N t_i) \prod_i^N t_i^{\alpha_i-1}\,\mathrm{d}^N\vec{t} = \underbrace{\frac{\prod_i^N \Gamma(\alpha_i)}{\Gamma(\sum_i^N \alpha_i)}}_{\Delta(\vec{\alpha})} \int_0^1 f(\tau)\tau^{(\sum_i^N \alpha_i)-1}\,\mathrm{d}\tau$$

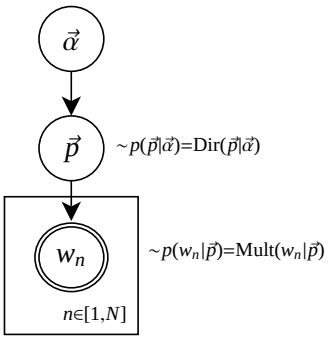

Fig. 4. Bayesian network of the Dirichlet–multinomial unigram model.

models (Markov random fields) and mixed models. By only considering the most relevant dependency relations, inference calculations are considerably simplified – compared to assuming dependency between all variables, which is exponentially complex w.r.t. their number.

A Bayesian network forms a directed acyclical graph (DAG) with nodes that correspond to random variables and edges that correspond to conditional probability distributions, where the condition variable at the origin of an edge is called a parent node and the dependent variable at the end of the edge a child node. Bayesian networks distinguish between evidence nodes, which correspond to variables that are observed or assumed observed, and hidden nodes, which correspond to latent variables.

In many models, replications of nodes exist that share parents and/or children, e.g., to account for multiple values or mixture components. Such replications can be denoted by plates, which surround the subset of nodes and have a replication count or a set declaration of the index variable at the lower right corner.

All elements of the graphical language can be seen in the Dirichlet–multinomial model shown in the last section whose corresponding BN is shown in Fig. 4. The double circle around the variable $\vec{w}=\{w_n\}$ denotes an evidence node, i.e., a variable that is (assumed as) observed, and the surrounding plate indicates the N i.i.d. samples. The unknown variables $\vec{p}$ and $\vec{\alpha}$ can be distinguished into a multivariate parameter $\vec{\alpha}$ and a hidden variable $\vec{p}$.

4.2 Conditional independence and exchangeability

Bayesian networks efficiently encode the dependency structure between random variables, which can be determined from the topology of the graph. Within this topology, the relevant indepencence property is *conditional* independence: Two variables X and Y are conditionally independent given a condition Z, symbolically $X \perp\!\!\!\perp Y|Z$, if $p(X, Y|Z) = p(X|Z) \cdot p(Y|Z)$. A verbal explanation of conditional independence is that

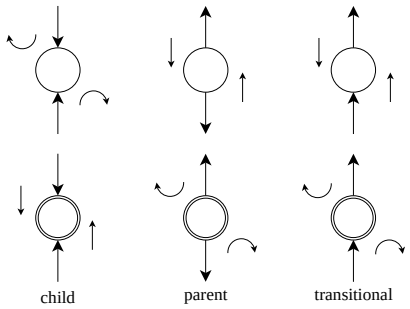

Fig. 5. Rules for the Bayes Ball method (after [Murp01]).

knowing Z, any information about the variable X does not add to the information about Y and vice versa. Here information can consist either of observations or parameters.

Markov conditions. In a Bayesian network, there are two general rules for the conditional independence of a node. The first is based on the *Markov blanket*: a subgraph of the BN defined as the set of a node's parents, its children, and its children's parents (co-parents). The condition states that a node, X_i, is conditionally independent of all other nodes, $X_{\neg i}$, given its Markov blanket, $B(X_i)$: $X_i \perp\!\!\!\perp X_{\neg i} | B(X_i)$.

The second rule refers to the set of *non-descendants* of a node: In a sequence of all BN nodes that ensures no node appears before any of its parents (*topological ordering*), all predecessors of a node that are not its parents are its non-descendants. The rule states that a node, X_i, is always conditionally independent of its non-descendants, $N(X_i)$, given its parents, $P(X_i)$: $X_i \perp\!\!\!\perp N(X_i) | P(X_i)$.

Bayes ball. To determine conditional independence between any nodes $X \perp\!\!\!\perp Y|Z$ in a BN, a straight-forward method is called "Bayes ball", which attempts to propagate a message (the Bayes ball) from X to Y, given observations for node Z [Shac88,Murp01]: $X \perp\!\!\!\perp Y|Z$ is true if and only if (iff) there is no way to pass the ball from X to Y, with the rules given in Fig. 5 where the double circles correspond to observed or given variables. The absence of a path from X to Y given Z makes these nodes *d-separated* by Z.

Summarised, the rules of Bayes ball state that child nodes block propagation iff they are hidden while parent and transitional nodes block propagation iff they are given or observed. For example, observations $\vec{w}$ and hyperparameters $\vec{\alpha}$ in Fig. 4 are conditionally independent given the parameters $\vec{p}$ (transitional node). The method also applies to sets of nodes $\{X_i\} \perp\!\!\!\perp \{Y_j\} | \{Z_k\}$, and conditional independence holds if all pairs (X_i, Y_j) are d-separated given the set of nodes $\{Z_k\}$, i.e., no Bayes ball path exists.

Exchangeability. An independence relation stronger than conditional independence and important in Bayesian statistics is that of exchangeability. Any finite sequence of r.v.s $\{X_n\}_n$ is referred to as exchangeable iff its joint distribution is invariant to any permutation $\mathrm{Perm}(n)$ of its order: $p(\{X_n\}_{n=1}^N) = p(\{X_{\mathrm{Perm}(n)}\}_{n=1}^N)$. For an infinite sequence, this is required of any finite subsequence, leading to infinite exchangeability.

The importance of exchangeability is motivated by de Finetti's theorem[15], which states that the joint distribution of an infinitely exchangeable sequence of random variables is equivalent to sampling a random parameter from some prior distribution and subsequently sampling i.i.d. random variables, conditioned on that random parameter [BNJ03]. The joint distribution then is $p(\{x_m\}_{m=1}^M) = \prod_{m=1}^M p(x_m|\vartheta)$.

In the Bayesian network graphical language, exchangebility given a parent variable is the condition to apply the plates notation, and variables can be assumed drawn i.i.d. given the parent. In Bayesian text modelling, exchangeability corresponds to the bag-of-words assumption.

4.3 Generative models

The advantage of Bayesian networks is that they provide an often intuitive description of an observed phenomenon as a so-called generative process, which states how the observations could have been generated by realisations of r.v.s (samples) and their propagation along the directed edges of the network. Variable dependencies and edges can often be justified by causal relationships which re-enact a real phenomenon or are used as a artificial variables.

For the simple case of the Dirichlet–multinomial model, the generative process of a unigram (word) looks as follows:

$$\vec{p} \sim \mathrm{Dir}(p|\alpha) \tag{53}$$

$$w \sim \mathrm{Mult}(w|\vec{p}) \tag{54}$$

This means, a vector of parameters $\vec{p}$ is sampled from a Dirichlet distribution, and afterwards a word w is sampled from the multinomial with parameters $\vec{p}$. The task of Bayesian inference is to "invert" generative processes and "generate" parameter values from given observations, trying to cope with any hidden variables. For the example model, this has been shown in Eq. 52, where the hidden variable $\vec{p}$ was handled by integrating it out. However, only in special cases is it possible to derive the complete posterior this way, and in the next section we will see how inference in a more complex model like LDA can be done.

5 Latent Dirichlet allocation

Latent Dirichlet allocation (LDA) by Blei et al. [BNJ02] is a probabilistic generative model that can be used to estimate the properties of multinomial observations by unsupervised learning. With respect to text modelling, LDA is a method to perform so-called latent semantic analysis (LSA). The intuition behind LSA is to find the latent structure of "topics" or "concepts" in a text corpus, which captures the meaning of the text that is imagined to be obscured by "word choice" noise. The term latent semantic analysis has been coined by Deerwester et al. [DDL+90] who empirically showed that the co-occurrence structure of terms in text documents can be used to recover this latent

[15] De Finetti considered binary variables, Hewitt and Savage [HeSa55] generalised this to arbitrary r.v.s $X_i \in \mathcal{X}$ relevant here.

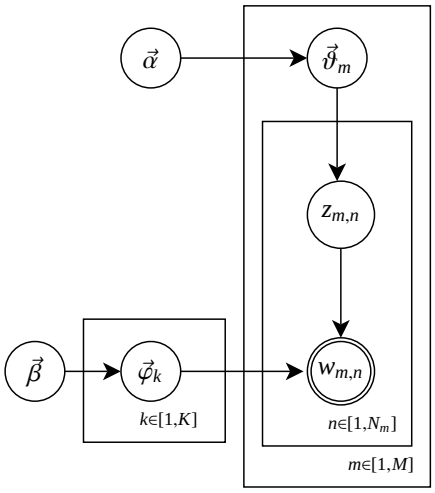

Fig. 6. Bayesian network of latent Dirichlet allocation.

topic structure, notably without any usage of background knowledge. In turn, latent-topic representations of text allow modelling of linguistic phenomena like synonymy and polysemy. This allows information retrieval systems to represent text in a way suitable for matching user needs (queries) with content items on a meaning level rather than by lexical congruence.

LDA is a model closely linked to the probabilistic latent semantic analysis (PLSA) by Hofmann [Hofm99], an application of the latent aspect method to the latent semantic analysis task. More specifically, LDA extends PLSA method by defining a complete generative process [BNJ02], and Girolami and Kaban showed that LDA with a uniform prior Dir(1) is a full Bayesian estimator for the same model for which PLSA provides an ML or MAP estimator [GiKa03].

5.1 Mixture modelling

LDA is a mixture model, i.e., it uses a convex combination of a set of component distributions to model observations. A convex combination is a weighted sum whose weighting proportion coefficients sum to one. In LDA, a word w is generated from a convex combination of topics z. In such a mixture model, the probability that a word w instantiates term t is:

$$p(w{=}t) = \sum_k p(w{=}t|z{=}k)p(z{=}k), \quad \sum_k p(z{=}k) = 1 \tag{55}$$

where each mixture component $p(w{=}t|z{=}k)$ is a multinomial distribution over terms (cf. the unigram model above) that corresponds to one of the latent topics $z{=}k$ of the text corpus. The mixture proportion consists of the topic probabilities $p(z{=}k)$. However,

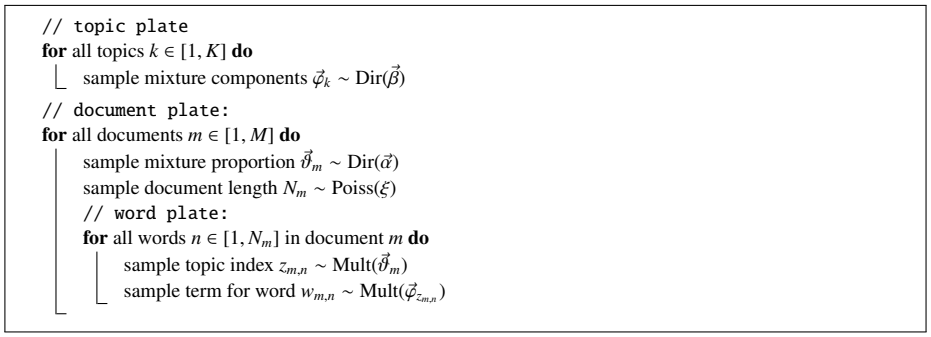

Fig. 7. Generative model for latent Dirichlet allocation.

LDA goes a step beyond a global topic proportion and conditions the topic probabilities on the document a word belongs to. Based on this, we can formulate the main objectives of LDA inference: to find (1) the term distribution $p(t|z{=}k) = \vec{\varphi}_k$ for each topic k and (2) the topic distribution $p(z|d{=}m) = \vec{\vartheta}_m$ for each document m. The estimated parameter sets $\underline{\Phi} = \{\vec{\varphi}_k\}_{k=1}^{K}$ and $\underline{\Theta} = \{\vec{\vartheta}_m\}_{m=1}^{M}$ are the basis for latent-semantic representation of words and documents.

5.2 Generative model

To derive an inference strategy, we view LDA as a generative process. Consider the Bayesian network of LDA shown in Fig. 6. This can be interpreted as follows: LDA generates a stream of observable words $w_{m,n}$, partitioned into documents $\vec{w}_m$. For each of these documents, a topic proportion $\vec{\vartheta}_m$ is drawn, and from this, topic-specific words are emitted. That is, for each word, a topic indicator $z_{m,n}$ is sampled according to the document-specific mixture proportion, and then the corresponding topic-specific term distribution $\vec{\varphi}_{z_{m,n}}$ used to draw a word. The topics $\vec{\varphi}_k$ are sampled once for the entire corpus.

Because LDA leaves flexibility to assign a different topic to every observed word (and a different proportion of topics for every document), the model is not only referred to as a mixture model, but in fact as an admixture model. In genetics, admixture refers to a mixture whose components are itself mixtures of different features. Bayesian modelling of admixture for discrete data was notably done by Pritchard et al. [PSD00] to model population genetics even before LDA was proposed for text. The complete (annotated) generative process [BNJ02] is presented in Fig. 7 while Fig. 8 gives a list of all involved quantities.

5.3 Likelihoods

Looking at the topology of the Bayesian network, we can specify the complete-data likelihood of a document, i.e., the joint distribution of all known and hidden variables

M	number of documents to generate (const scalar).
K	number of topics / mixture components (const scalar).
V	number of terms t in vocabulary (const scalar).
$\vec{\alpha}$	hyperparameter on the mixing proportions (K-vector or scalar if symmetric).
$\vec{\beta}$	hyperparameter on the mixture components (V-vector or scalar if symmetric).
$\vec{\vartheta}_m$	parameter notation for $p(z\|d{=}m)$, the topic mixture proportion for document m. One proportion for each document, $\underline{\Theta} = \{\vec{\vartheta}_m\}_{m=1}^{M}$ ($M \times K$ matrix).
$\vec{\varphi}_k$	parameter notation for $p(t\|z{=}k)$, the mixture component of topic k. One component for each topic, $\underline{\Phi} = \{\vec{\varphi}_k\}_{k=1}^{K}$ ($K \times V$ matrix).
N_m	document length (document-specific), here modelled with a Poisson distribution [BNJ02] with constant parameter ξ.
$z_{m,n}$	mixture indicator that chooses the topic for the nth word in document m.
$w_{m,n}$	term indicator for the nth word in document m.

Fig. 8. Quantities in the model of latent Dirichlet allocation

given the hyperparameters:

$$p(\vec{w}_m, \vec{z}_m, \vec{\vartheta}_m, \underline{\Phi}|\vec{\alpha}, \vec{\beta}) = \overbrace{\underbrace{\prod_{n=1}^{N_m} p(w_{m,n}|\vec{\varphi}_{z_{m,n}}) p(z_{m,n}|\vec{\vartheta}_m)}_{\text{word plate}} \cdot p(\vec{\vartheta}_m|\vec{\alpha})}^{\text{document plate (1 document)}} \cdot \underbrace{p(\underline{\Phi}|\vec{\beta})}_{\text{topic plate}} . \tag{56}$$

To specify this distribution is simple and useful as a basis for other derivations. So the probability that a word $w_{m,n}$ instantiates a particular term t given the LDA parameters is obtained by marginalising $z_{m,n}$ from the word plate and omitting the parameter distributions:

$$p(w_{m,n}{=}t|\vec{\vartheta}_m, \underline{\Phi}) = \sum_{k=1}^{K} p(w_{m,n}{=}t|\vec{\varphi}_k) p(z_{m,n}{=}k|\vec{\vartheta}_m) , \tag{57}$$

which is just the mixture model in Eq. 55 with document-specific mixture weights. The likelihoods of a document $\vec{w}_m$ and of the corpus $\mathcal{W} = \{\vec{w}_m\}_{m=1}^{M}$ are just the joint likelihoods of the independent events of the token observations $w_{m,n}$:

$$p(\mathcal{W}|\underline{\Theta}, \underline{\Phi}) = \prod_{m=1}^{M} p(\vec{w}_m|\vec{\vartheta}_m, \underline{\Phi}) = \prod_{m=1}^{M} \prod_{n=1}^{N_m} p(w_{m,n}|\vec{\vartheta}_m, \underline{\Phi}) . \tag{58}$$

5.4 Inference via Gibbs sampling

Although latent Dirichlet allocation is still a relatively simple model, exact inference is generally intractable. The solution to this is to use approximate inference algorithms, such as mean-field variational expectation maximisation [BNJ02], expectation propagation [MiLa02], and Gibbs sampling [Grif02,GrSt04,PSD00].

Gibbs sampling is a special case of Markov-chain Monte Carlo (MCMC) simulation [MacK03,Liu01] and often yields relatively simple algorithms for approximate inference in high-dimensional models such as LDA. Therefore we select this approach

and present a derivation that is more detailed than the original one by Griffiths and Steyvers [Grif02,GrSt04]. An alternative approach to Gibbs sampling in an LDA-like model is due to Pritchard et al. [PSD00] that actually pre-empted LDA in its interpretation of admixture modelling and formulated a direct Gibbs sampling algorithm for a model comparable to Bayesian PLSA [16].

MCMC methods can emulate high-dimensional probability distributions $p(\vec{x})$ by the stationary behaviour of a Markov chain. This means that one sample is generated for each transition in the chain after a stationary state of the chain has been reached, which happens after a so-called "burn-in period" that eliminates the influence of initialisation parameters. Gibbs sampling is a special case of MCMC where the dimensions x_i of the distribution are sampled alternately one at a time, conditioned on the values of all other dimensions, which we denote $\vec{x}_{\neg i}$. The algorithm works as follows:

1. choose dimension i (random or by permutation[17])
2. sample x_i from $p(x_i|\vec{x}_{\neg i})$.

To build a Gibbs sampler, the univariate conditionals (or full conditionals) $p(x_i|\vec{x}_{\neg i})$ must be found, which is possible using:

$$p(x_i|\vec{x}_{\neg i}) = \frac{p(\vec{x})}{p(\vec{x}_{\neg i})} = \frac{p(\vec{x})}{\int p(\vec{x})\,\mathrm{d}x_i} \text{ with } \vec{x} = \{x_i, \vec{x}_{\neg i}\} \tag{59}$$

For models that contain hidden variables $\vec{z}$, their posterior given the evidence, $p(\vec{z}|\vec{x})$, is a distribution commonly wanted. With Eq. 59, the general formulation of a Gibbs sampler for such latent-variable models becomes:

$$p(z_i|\vec{z}_{\neg i}, \vec{x}) = \frac{p(\vec{z}, \vec{x})}{p(\vec{z}_{\neg i}, \vec{x})} = \frac{p(\vec{z}, \vec{x})}{\int_Z p(\vec{z}, \vec{x})\,\mathrm{d}z_i}, \tag{60}$$

where the integral changes to a sum for discrete variables. With a sufficient number of samples $\tilde{\vec{z}}_r$, $r \in [1, R]$, the latent-variable posterior can be approximated using:

$$p(\vec{z}|\vec{x}) \approx \frac{1}{R}\sum_{r=1}^{R} \delta(\vec{z} - \tilde{\vec{z}}_r), \tag{61}$$

with the Kronecker delta $\delta(\vec{u})$ = {1 if $\vec{u}$=0; 0 otherwise}.

5.5 The collapsed LDA Gibbs sampler

To derive a Gibbs sampler for LDA, we apply the hidden-variable method from above. The hidden variables in our model are $z_{m,n}$, i.e., the topics that appear with the words of the corpus $w_{m,n}$. We do not need to include, i.e., can integrate out, the parameter sets $\underline{\Theta}$ and $\underline{\Phi}$ because they can be interpreted as statistics of the associations between the

[16] This work is lesser known in the text modelling field due to its application in genetics, which uses different notation and terminology.

[17] Liu [Liu01] calls these variants random-scan and systematic-scan Gibbs samplers.

Algorithm `LdaGibbs(`$\{\vec{w}\}, \alpha, \beta, K$`)`
Input: word vectors $\{\vec{w}\}$, hyperparameters α, β, topic number K
Global data: count statistics $\{n_m^{(k)}\}$, $\{n_k^{(t)}\}$ and their sums $\{n_m\}$, $\{n_k\}$, memory for full conditional array $p(z_i|\cdot)$
Output: topic associations $\{\vec{z}\}$, multinomial parameters $\underline{\Phi}$ and $\underline{\Theta}$, hyperparameter estimates α, β
`// initialisation`
zero all count variables, $n_m^{(k)}, n_m, n_k^{(t)}, n_k$
for all documents $m \in [1, M]$ **do**
  for all words $n \in [1, N_m]$ in document m **do**
    sample topic index $z_{m,n}{=}k \sim \mathrm{Mult}(1/K)$
    increment document–topic count: $n_m^{(k)}$ += 1
    increment document–topic sum: n_m += 1
    increment topic–term count: $n_k^{(t)}$ += 1
    increment topic–term sum: n_k += 1
`// Gibbs sampling over burn-in period and sampling period`
while not finished **do**
  for all documents $m \in [1, M]$ **do**
    for all words $n \in [1, N_m]$ in document m **do**
      `// for the current assignment of` k `to a term` t `for word` $w_{m,n}$`:`
      decrement counts and sums: $n_m^{(k)} -{=} 1; n_m -{=} 1; n_k^{(t)} -{=} 1; n_k -{=} 1$
      `// multinomial sampling acc. to Eq. 78 (decrements from previous step):`
      sample topic index $\tilde{k} \sim p(z_i|\vec{z}_{\neg i}, \vec{w})$
      `// for the new assignment of` $z_{m,n}$ `to the term` t `for word` $w_{m,n}$`:`
      increment counts and sums: $n_m^{(\tilde{k})}$ += 1; n_m += 1; $n_{\tilde{k}}^{(t)}$ += 1; $n_{\tilde{k}}$ += 1
  `// check convergence and read out parameters`
  if converged and L sampling iterations since last read out **then**
    `// the different parameters read outs are averaged.`
    read out parameter set $\underline{\Phi}$ according to Eq. 81
    read out parameter set $\underline{\Theta}$ according to Eq. 82

Fig. 9. Gibbs sampling algorithm for latent Dirichlet allocation

observed $w_{m,n}$ and the corresponding $z_{m,n}$, the state variables of the Markov chain. The strategy of integrating out some of the parameters for model inference is often referred to as "collapsed" [Neal00] or Rao-Blackwellised [CaRo96] approach, which is often used in Gibbs sampling.[18]

The target of inference is the distribution $p(\vec{z}|\vec{w})$, which is directly proportional to the joint distribution

$$p(\vec{z}|\vec{w}) = \frac{p(\vec{z}, \vec{w})}{p(\vec{w})} = \frac{\prod_{i=1}^{W} p(z_i, w_i)}{\prod_{i=1}^{W} \sum_{k=1}^{K} p(z_i{=}k, w_i)} \tag{62}$$

where the hyperparameters are omitted. This distribution covers a large space of discrete random variables, and the difficult part for evaluation is its denominator, which represents a summation over K^W terms. At this point, the Gibbs sampling procedure comes into play. In our setting, the desired Gibbs sampler runs a Markov chain that

[18] Cf. the non-collapsed strategy pursued in the similar admixture model of [PSD00].

uses the full conditional $p(z_i|\vec{z}_{\neg i}, \vec{w})$ in order to simulate $p(\vec{z}|\vec{w})$. We can obtain the full conditional via the hidden-variable approach by evaluating Eq. 60, which requires to formulate the joint distribution.

Joint distribution. In LDA, this joint distribution can be factored:

$$p(\vec{w}, \vec{z}|\vec{\alpha}, \vec{\beta}) = p(\vec{w}|\vec{z}, \vec{\beta}) p(\vec{z}|\vec{\alpha}), \tag{63}$$

because the first term is independent of $\vec{\alpha}$ (conditional independence $\vec{w} \perp\!\!\!\perp \vec{\alpha}|\vec{z}$), and the second term is independent of $\vec{\beta}$. Both elements of the joint distribution can now be handled separately. The first term, $p(\vec{w}|\vec{z})$, can be derived from a multinomial on the observed word counts given the associated topics:

$$p(\vec{w}|\vec{z}, \underline{\Phi}) = \prod_{i=1}^{W} p(w_i|z_i) = \prod_{i=1}^{W} \varphi_{z_i, w_i}. \tag{64}$$

That is, the W words of the corpus are observed according to independent multinomial trials[19] with parameters conditioned on the topic indices z_i. We can now split the product over words into one product over topics and one over the vocabulary, separating the contributions of the topics:

$$p(\vec{w}|\vec{z}, \underline{\Phi}) = \prod_{k=1}^{K} \prod_{\{i:z_i=k\}} p(w_i{=}t|z_i{=}k) = \prod_{k=1}^{K} \prod_{t=1}^{V} \varphi_{k,t}^{n_k^{(t)}}, \tag{65}$$

where we use the notation $n_k^{(t)}$ to denote the number of times that term t has been observed with topic k. The target distribution $p(\vec{w}|\vec{z}, \vec{\beta})$ is obtained by integrating over $\underline{\Phi}$, which can be done componentwise using Dirichlet integrals within the product over z:

$$p(\vec{w}|\vec{z}, \vec{\beta}) = \int p(\vec{w}|\vec{z}, \underline{\Phi})\ p(\underline{\Phi}|\vec{\beta})\ \mathrm{d}\underline{\Phi} \tag{66}$$

$$= \int \prod_{z=1}^{K} \frac{1}{\Delta(\vec{\beta})} \prod_{t=1}^{V} \varphi_{z,t}^{n_z^{(t)}+\beta_t-1}\, \mathrm{d}\vec{\varphi}_z \tag{67}$$

$$= \prod_{z=1}^{K} \frac{\Delta(\vec{n}_z + \vec{\beta})}{\Delta(\vec{\beta})}, \quad \vec{n}_z = \{n_z^{(t)}\}_{t=1}^{V}. \tag{68}$$

This can be interpreted as a product of K Dirichlet–multinomial models (cf. Eq. 52), representing the corpus by K separate "topic texts".

Analogous to $p(\vec{w}|\vec{z}, \vec{\beta})$, the topic distribution $p(\vec{z}|\vec{\alpha})$ can be derived, starting with the conditional and rewriting its parameters into two products, separating the contributions of the documents:

$$p(\vec{z}|\underline{\Theta}) = \prod_{i=1}^{W} p(z_i|d_i) = \prod_{m=1}^{M} \prod_{k=1}^{K} p(z_i{=}k|d_i{=}m) = \prod_{m=1}^{M} \prod_{k=1}^{K} \vartheta_{m,k}^{n_m^{(k)}}, \tag{69}$$

[19] Omitting the multinomial coefficient corresponds to the bag-of-words assumption that ignores any sequential information of the document words.

where the notation d_i refers to the document a word i belongs to and $n_m^{(k)}$ refers to the number of times that topic k has been observed with a word of document m. Integrating out $\underline{\Theta}$, we obtain:

$$p(\vec{z}|\vec{\alpha}) = \int p(\vec{z}|\underline{\Theta})\; p(\underline{\Theta}|\vec{\alpha})\; \mathrm{d}\underline{\Theta} \tag{70}$$

$$= \int \prod_{m=1}^{M} \frac{1}{\Delta(\vec{\alpha})} \prod_{k=1}^{K} \vartheta_{m,k}^{n_m^{(k)}+\alpha_k-1}\, \mathrm{d}\vec{\vartheta}_m \tag{71}$$

$$= \prod_{m=1}^{M} \frac{\Delta(\vec{n}_m + \vec{\alpha})}{\Delta(\vec{\alpha})}, \quad \vec{n}_m = \{n_m^{(k)}\}_{k=1}^{K}. \tag{72}$$

The joint distribution therefore becomes:

$$p(\vec{z}, \vec{w}|\vec{\alpha}, \vec{\beta}) = \prod_{z=1}^{K} \frac{\Delta(\vec{n}_z + \vec{\beta})}{\Delta(\vec{\beta})} \cdot \prod_{m=1}^{M} \frac{\Delta(\vec{n}_m + \vec{\alpha})}{\Delta(\vec{\alpha})}. \tag{73}$$

Full conditional. From the joint distribution, we can derive the full conditional distribution for a word token with index i=(m, n), i.e., the update equation from which the Gibbs sampler draws the hidden variable. Using the chain rule and noting that $\vec{w} = \{w_i{=}t, \vec{w}_{\neg i}\}$ and $\vec{z} = \{z_i{=}k, \vec{z}_{\neg i}\}$ yields:[20]

$$p(z_i{=}k|\vec{z}_{\neg i}, \vec{w}) = \frac{p(\vec{w}, \vec{z})}{p(\vec{w}, \vec{z}_{\neg i})} = \frac{p(\vec{w}|\vec{z})}{p(\vec{w}_{\neg i}|\vec{z}_{\neg i})p(w_i)} \cdot \frac{p(\vec{z})}{p(\vec{z}_{\neg i})} \tag{74}$$

$$\propto \frac{\Delta(\vec{n}_z + \vec{\beta})}{\Delta(\vec{n}_{z,\neg i} + \vec{\beta})} \cdot \frac{\Delta(\vec{n}_m + \vec{\alpha})}{\Delta(\vec{n}_{m,\neg i} + \vec{\alpha})} \tag{75}$$

$$= \frac{\Gamma(n_k^{(t)} + \beta_t)\; \Gamma(\sum_{t=1}^{V} n_{k,\neg i}^{(t)} + \beta_t)}{\Gamma(n_{k,\neg i}^{(t)} + \beta_t)\; \Gamma(\sum_{t=1}^{V} n_k^{(t)} + \beta_t)} \cdot \frac{\Gamma(n_m^{(k)} + \alpha_k)\; \Gamma(\sum_{k=1}^{K} n_{m,\neg i}^{(k)} + \alpha_k)}{\Gamma(n_{m,\neg i}^{(k)} + \alpha_k)\; \Gamma(\sum_{k=1}^{K} n_m^{(k)} + \alpha_k)} \tag{76}$$

$$= \frac{n_{k,\neg i}^{(t)} + \beta_t}{\sum_{t=1}^{V} n_{k,\neg i}^{(t)} + \beta_t} \cdot \frac{n_{m,\neg i}^{(k)} + \alpha_k}{[\sum_{k=1}^{K} n_m^{(k)} + \alpha_k] - 1} \tag{77}$$

$$\propto \frac{n_{k,\neg i}^{(t)} + \beta_t}{\sum_{t=1}^{V} n_{k,\neg i}^{(t)} + \beta_t} (n_{m,\neg i}^{(k)} + \alpha_k) \tag{78}$$

where the counts $n_{\cdot,\neg i}^{(\cdot)}$ indicate that the token i is excluded from the corresponding document or topic[21] and the hyperparameters are omitted.[22]

[20] Eq. 74 uses the independence assumption $w_i \perp\!\!\!\perp \vec{z}_{\neg i}$ that stems from $z_i \perp\!\!\!\perp \vec{z}_{\neg i}$, and the constant $p(w_i)$ is omitted afterwards. Further, the denominator of the second fraction in Eq. 77 may be omitted because it is independent of k.

[21] This is equivalent to using Kronecker deltas on the counts: $n_{u,\neg i}^{(v)} = n_u^{(v)} - \delta(u{-}u_i)$ where u and v are placeholders for indices and u_i represents the association of the current token (document or topic).

[22] Alternative derivation strategies of LDA-type Gibbs samplers have been published in [Grif02] who works via $p(z_i|\vec{z}_{\neg i}, \vec{w}) \propto p(w_i|\vec{w}_{\neg i}, z)p(z_i|\vec{z}_{\neg i})$ and [MWC07] who use the chain rule via the joint token likelihood, $p(z_i|\vec{z}_{\neg i}, \vec{w}_{\neg i}) = p(z_i, w_i|\vec{z}_{\neg i}, \vec{w}_{\neg i})/p(w_i|\vec{z}_{\neg i}, \vec{w}_{\neg i}) \propto p(\vec{z}, \vec{w})/p(\vec{z}_{\neg i}, \vec{w}_{\neg i})$, which is similar to the approach taken here.

Multinomial parameters. Finally, we need to obtain the multinomial parameter sets $\underline{\Theta}$ and $\underline{\Phi}$ that correspond to the state of the Markov chain, $\vec{z}$. According to their definitions as multinomial distributions with Dirichlet prior, applying Bayes' rule on the component $z{=}k$ in Eq. 65 and m in Eq. 69 yields:[23]

$$p(\vec{\vartheta}_m|\vec{z}_m,\vec{\alpha}) = \frac{1}{Z_{\vartheta_m}} \prod_{n=1}^{N_m} p(z_{m,n}|\vec{\vartheta}_m) \cdot p(\vec{\vartheta}_m|\vec{\alpha}) = \mathrm{Dir}(\vec{\vartheta}_m|\vec{n}_m + \vec{\alpha}), \tag{79}$$

$$p(\vec{\varphi}_k|\vec{z},\vec{w},\vec{\beta}) = \frac{1}{Z_{\varphi_k}} \prod_{\{i:z_i=k\}} p(w_i|\vec{\varphi}_k) \cdot p(\vec{\varphi}_k|\vec{\beta}) = \mathrm{Dir}(\vec{\varphi}_k|\vec{n}_k + \vec{\beta}) \tag{80}$$

where $\vec{n}_m$ is the vector of topic observation counts for document m and $\vec{n}_k$ that of term observation counts for topic k. Using the expectation of the Dirichlet distribution, $\langle \mathrm{Dir}(\vec{a})\rangle = a_i / \sum_i a_i$, on these results yields:[24]

$$\varphi_{k,t} = \frac{n_k^{(t)} + \beta_t}{\sum_{t=1}^{V} n_k^{(t)} + \beta_t}, \tag{81}$$

$$\vartheta_{m,k} = \frac{n_m^{(k)} + \alpha_k}{\sum_{k=1}^{K} n_m^{(k)} + \alpha_k}. \tag{82}$$

Gibbs sampling algorithm. Using Eqs. 78, 81 and 82, the Gibbs sampling procedure in Fig. 9 can be run. The procedure itself uses only five larger data structures, the count variables $n_m^{(z)}$ and $n_z^{(t)}$, which have dimension $M \times K$ and $K \times V$ respectively, their row sums n_m and n_z with dimension M and K, as well as the state variable $z_{m,n}$ with dimension W.[25] The Gibbs sampling algorithm runs over the three periods: initialisation, burn-in and sampling. However, to determine the required lengths of the burn-in is one of the drawbacks with MCMC approaches. There are several criteria to check that the Markov chain has converged (see [Liu01]), and we manually check how well the parameters cluster semantically related words and documents for different corpora and use these values as estimates for comparable settings.

To obtain the resulting model parameters from a Gibbs sampler, several approaches exist. One is to just use only one read out, another is to average a number of samples, and often it is desirable to leave an interval of L iteration between subsequent read-outs to obtain decorrelated states of the Markov chain. This interval is often called "thinning interval" or sampling lag.

6 LDA hyperparameters

In Section 5, values of the Dirichlet parameters have been assumed to be known. These hyperparameters, however, significantly influence the behaviour of the LDA model, as

[23] Cf. Eq. 47.

[24] Alternatively, the parameters can be obtained by the predictive distribution of a topic $\tilde{z}{=}k$ for a given term $\tilde{w}{=}t$ associated with document m, given the state $\mathcal{M}$. Analogous to Eq. 78 but now with one token $\tilde{w}$ beyond the corpus $\vec{w}$, this yields $p(\tilde{z}{=}k|\tilde{w}{=}t, m; \mathcal{M}) = \varphi_{k,t} \cdot \vartheta_{m,k} / p(\tilde{w}{=}t)$.

[25] The sum n_m is just the document length.

can be seen for instance from Eqs. 68 and 72, as well as by observing the different shapes of the Dirichlet density: For K=2, this corresponds to the beta density plotted in Fig. 1. Typically, in LDA symmetric Dirichlet priors are used, which means that the a priori assumption of the model is that all topics have the same chance of being assigned to a document and all words (frequent and infrequent ones) have the same chance of being assigned to a topic. This section gives an overview of the meaning of the hyperparameters and suggests a method to estimate their values from data.

6.1 Interpretations

Dirichlet hyperparameters generally have a smoothing effect on multinomial parameters. Reducing this smoothing effect in LDA by lowering the values of α and β will result in more decisive topic associations, thus $\underline{\Theta}$ and $\underline{\Phi}$ will become sparser. Sparsity of $\underline{\Phi}$, controlled by β, means that the model prefers to assign few terms to each topic, which again may influence the number of topics that the model assumes to be inherent in the data. This is related to how "similar" words need to be (that is, how often they need to co-occur across different contexts[26]) to find themselves assigned to the same topic. That is, for sparse topics, the model will fit better to the data if K is set higher because the model is reluctant to assign several topics to a given term. This is one reason why in models that learn K, such as non-parametric Bayesian approaches [TJB+06], K strongly depends on the hyperparameters. Sparsity of $\underline{\Theta}$, controlled by α, means that the model prefers to characterise documents by few topics.

As the relationship between hyperparameters, topic number and model behaviour is a mutual one, it can be used for synthesis of models with specific properties, as well as for analysis of features inherent in the data. Heuristically, good model quality (see next section for analysis methods) has been reported for $\alpha = 50/K$ and $\beta = 0.01$ [GrSt04]. On the other hand, learning α and β from the data can be used to increase model quality (w.r.t. to the objective of the estimation method), given the number of topics K. Further, hyperparameter estimates may reveal specific properties of the data set modelled. The estimate for α is an indicator of how different documents are in terms of their (latent) semantics, and the estimate for β suggests how large the groups of commonly co-occurring words are. However, the interpretation of estimated hyperparameters is not always simple, and the influence of specific constellations of document content has not yet been thoroughly investigated. In the following, we consider estimation of α, which is analogous to that of β.

6.2 Estimation

Several approaches to learn Dirichlet parameter vectors $\vec{\alpha}$ from data are known, but unfortunately no exact closed-form solution exists, nor is there a conjugate prior distribution for straight-forward Bayesian inference. The most exact approaches are iterative approximations. For a comprehensive overview, see [Mink00]. In fact, the best way of learning Dirichlet parameters would be to use the information already available from

[26] Latent topics often result from higher-order co-occurrence, i.e., t_1 co-occurring with t_2 that co-occurrs with t_3 represents a second-order co-occurrence between t_1 and t_3, and so on.

the (collapsed) Gibbs sampler (see Eq. 78), i.e., the count statistics of the topic associations instead of the multinomial parameters $\underline{\Theta}$ and $\underline{\Phi}$, which are integrated out. This means hyperparameters are best estimated as parameters of the Dirichlet–multinomial distribution (see Eq. 52).

For unconstrained vectorial Dirichlet parameters, a simple and stable fixed-point iteration for a maximum likelihood estimator is:[27]

$$\alpha_k \leftarrow \frac{\alpha_k \left[\left(\sum_{m=1}^{M} \Psi(n_{m,k} + \alpha_k)\right) - M\Psi(\alpha_k)\right]}{\left[\sum_{m=1}^{M} \Psi(n_m + \sum_k \alpha_k)\right] - M\Psi(\sum_k \alpha_k)} \tag{83}$$

where $\Psi(x)$ is the digamma function, the derivative of $\log \Gamma(x)$. The estimation can be initialised with a coarse-grained heuristic or estimate and converges within few iterations.

For symmetric Dirichlet distributions more common for LDA (where topics and terms are considered exchangeable), estimators for α and β that work well in Gibbs samplers are not explicitly found in the literature. Here the fact can be used that the parameter is just the precision of the Dirichlet divided by K:[28]

$$\alpha \leftarrow \frac{\alpha \left[\left(\sum_{m=1}^{M} \sum_{k=1}^{K} \Psi(n_{m,k} + \alpha)\right) - MK\Psi(\alpha)\right]}{K\left[\left(\sum_{m=1}^{M} \Psi(n_m + K\alpha)\right) - M\Psi(K\alpha)\right]} \,. \tag{84}$$

Extensions. The ML estimators described may be augmented to MAP estimators by placing a prior on the hyperparameter, for instance a gamma distribution. This requires to extend the derivation of [Mink00] by maximising with the prior distribution added to the likelihood, following Eq. 13. Moreover, sampling the hyperparameter using MCMC methods may be considered, which allows a fully Bayesian approach. The sampling distribution then is $p(\alpha|\vec{z}) \propto p(\vec{z}|\alpha)p(\alpha)$, which is simulated for instance using adaptive rejection Metropolis sampling (ARMS [GBT95]) or, if $p(\alpha|\vec{z})$ is log-concave ($[\log f]'' < 0$), adaptive rejection sampling (ARS [GiWi92]) that omits the computationally expensive Metropolis step.

7 Analysing topic models

Topic models such as LDA estimate soft associations between latent topics and observed entities, i.e., words, documents, but in model extensions also authors etc. These associations are the basis for a number of operations relevant to information processing and language modelling. In this section, we outline methods to use the topic structure of a given corpus in order (1) to estimate the topic structure of unseen documents (querying), (2) to estimate the quality of the clustering implied by the estimated topics and (3) to infer new associations on the basis of the estimated ones, e.g., the similarity between words or between documents or their authors. For this, the exemplary case of LDA is used, which provides information about the topics present in documents – the parameter set $\underline{\Theta}$ –, and the terms associated with these topics – the parameter set $\underline{\Phi}$.

[27] This is Eq. 55 in [Mink00] with a derivation in its Appendix B.

[28] This corresponds to Eq. 83 in [Mink00] with additional division by K.

7.1 Querying

Topic models provide at least two methods to retrieve documents similar to a query document, i.e., perform ranking of a given document set: (1) via similarity analysis of document parameters and (2) via the predictive document likelihood. Both methods depend on the estimation of the topics of the query document or documents.

Query sampling. A query is, like any other document, simply a vector of words $\tilde{\vec{w}}$, and we can find matches with known documents by estimating the posterior distribution of topics $\tilde{\vec{z}}$ given the word vector of the query $\tilde{\vec{w}}$ and the LDA model $\mathcal{M}$ and calculating the document-specific parameters $\tilde{\vec{\vartheta}}_m$ from the statistics of word–topic associations $\{\tilde{\vec{w}}, \tilde{\vec{z}}\}$ with the corresponding distribution $p(\tilde{\vec{z}}|\tilde{\vec{w}}; \mathcal{M})$.

In order to find these associations, we can follow the approach of [Hofm99] or [SSR+04] to run the inference algorithm on the new document exclusively. Inference for this corresponds to Eq. 78 with the difference that (1) the state of the Gibbs sampler can be run with the estimated parameters $\underline{\Phi}$ and hyperparameters α held fixed and (2) the parameters $\underline{\tilde{\Theta}}$ now cover the query document(s). Consequently, an LDA model $\mathcal{M}$ needs to contain the trained topic distributions $\underline{\Phi}$ as well as hyperparameter α.

We first initialise the algorithm by randomly assigning topics to words and then perform a number of loops through the Gibbs sampling update (locally for the words i of $\tilde{m}$):

$$p(\tilde{z}_i{=}k|\tilde{w}_i{=}t, \tilde{\vec{z}}_{\neg i}, \tilde{\vec{w}}_{\neg i}; \mathcal{M}) \propto \varphi_{k,t} \; (n^{(k)}_{\tilde{m},\neg i} + \alpha_k) \; . \tag{85}$$

This equation gives a colourful example of the workings of Gibbs posterior sampling: Word–topic associations $\varphi_{k,t}$ estimated highly will dominate the multinomial masses compared to the contributions of $n^{(k)}_{\tilde{m}}$, which are initialised randomly and therefore unlikely to be clustered. Consequently, on repeatedly sampling from the distribution and updating of $n^{(k)}_{\tilde{m}}$, the masses of topic–word associations are propagated into document–topic associations. Note the smoothing influence of the Dirichlet hyperparameter.

After sampling, applying Eq. 82 yields the topic distribution for the unknown document:

$$\vartheta_{\tilde{m},k} = \frac{n^{(k)}_{\tilde{m}} + \alpha_k}{\sum_{k=1}^{K} n^{(k)}_{\tilde{m}} + \alpha_k}. \tag{86}$$

This querying procedure is applicable for complete collections of unknown documents, which is done by letting $\tilde{m}$ range over the unknown documents.

Similarity ranking. In the similarity method, the topic distribution of the query document(s) is estimated and appropriate similarity measures permit ranking. As the distribution over topics $\vec{\vartheta}_{\tilde{m}}$ now is in the same form as the rows of $\underline{\Theta}$, we can compare the query to the documents of the corpus. A simple measure is the Kullback-Leibler divergence [KuLe51], which is defined between two discrete random variables X and Y, as:

$$D_{\mathrm{KL}}(X\|Y) = \sum_{n=1}^{N} p(X{=}n) \; [\log_2 p(X{=}n) - \log_2 p(Y{=}n)] \tag{87}$$

The KL divergence can be interpreted as the difference between the cross entropy of $H(X||Y) = -\sum_n p(X{=}n) \log_2 p(Y{=}n)$ and the entropy of X, $H(X) = -\sum_n p(X{=}n) \log_2 p(X{=}n)$, i.e., it is the information that knowledge of Y adds to the knowledge of X. Thus only if both distributions X and Y are equal, the KL divergence becomes zero.

However, the KL divergence is not a distance measure proper because it is not symmetric. Thus alternatively, a smoothed, symmetrised extension, the Jensen-Shannon distance, can be used:

$$D_{\mathrm{JS}}(X||Y) = \frac{1}{2}[D_{\mathrm{KL}}(X||M) + D_{\mathrm{KL}}(Y||M)] \tag{88}$$

with the averaged variable $M = \frac{1}{2}(X + Y)$.

Predictive likelihood ranking. The second approach to ranking is to calculate a predictive likelihood that the document (with index m) of the corpus could be generated by the query (symbolically indexed as $\tilde{m}$). One possibility to formulate a predictive likelihood is to apply Bayes' rule to the document-specific parameters:[29]

$$p(m|\tilde{m}) = \sum_{k=1}^{K} p(m|z{=}k)p(z{=}k|\tilde{m}) \tag{89}$$

$$= \sum_{k=1}^{K} \frac{p(z{=}k|m)p(m)}{p(z{=}k)} p(z{=}k|\tilde{m}) \tag{90}$$

$$= \sum_{k=1}^{K} \vartheta_{m,k} \frac{n_m}{n_k} \vartheta_{\tilde{m},k} \tag{91}$$

where we assume the probability of the document m to be proportional to its length n_m but could in principle use any other prior probability. Intuitively, Eq. 91 is a weighted scalar product between topic vectors that penalises short documents and strong topics.

Retrieval. Because query results provide a ranking over the document set, querying of topic models may be used for information retrieval. This requires some additional considerations, though. By itself, the capabilities of topic models to map semantically similar items of different literal representation (synonymy) closely in topic-space and represent multiple semantics of literals (polysemy) comes at the price that results are less precise in a literal sense (while providing larger recall). Depending on the kind relevance expected from the query results, combination of latent-topic query results with other retrieval approaches may be useful, cf. [WeCr06].

Another aspect of topic-based querying is that different strategies of query construction are useful. Clearly, a Boolean approach to query construction will not suffice, but rather a strategy comparable with vector-space models can be used. More specifically, for effective retrieval queries can be constructed in a way that more and more precisely narrows down the topic distribution considered relevant, which raises issues of query refinement and expansion and interactive search processes [BaRi99].

[29] We use the probabilities of a document $p(m) = n_m/W$ and a topic $p(z{=}k) = n_k/W$ with $W = \sum_m n_m = \sum_k n_k$. Note the difference between $p(m)$ and $p(\vec{w}_m)$: $p(m)$ is the likelihood to choose document m as a whole from the corpus, whereas $p(\vec{w}_m)$ is the likelihood of a set of word tokens $\{w_i\}$ being observed in document m.

7.2 Clustering

Often it is of importance to cluster documents or terms. As mentioned above, the LDA model already provides a soft clustering of the documents and of the terms of a corpus by associating them to topics. To use this clustering information requires the evaluation of similarity, and in the last section, the similarity between a query document and the corpus documents was computed using the Kullback Leibler divergence. This measure can be applied to the distributions of words over topics as well as to the distribution of topics over documents in general, which reveals the internal similarity pattern of the corpus according to its latent semantic structure.

In addition to determining similarities, the evaluation of clustering quality is of particular interest for topic models like LDA. In principle, evaluation can be done by subjective judgement of the estimated word and document similarities. A more objective evaluation, however, is the comparison of the estimated model to an a priori categorisation for a given corpus as a reference[30]. Among the different methods to compare clusterings, we will show the Variation of Information distance (VI-distance) that is able to calculate the distance between soft or hard clusterings of different numbers of classes and therefore provides maximum flexibility of application.

The VI distance measure has been proposed by Meila [Meil03], and it assumes two distributions over classes for each document: $p(c{=}j|d_m)$ and $p(z{=}k|d_m)$ with class labels (or topics) $j \in [1, J]$ and $k \in [1, K]$. Averaging over the corpus yields the class probabilities $p(c{=}j) = 1/M \sum_m p(c{=}j|d_m)$ and $p(z{=}k) = 1/M \sum_m p(z{=}k|d_m)$.

Similar clusterings tend to have co-occurring pairs $(c{=}j, z{=}k)$ of high probability $p(\cdot|d_m)$. Conversely, dissimilarity corresponds to independence of the class distributions for all documents, i.e., $p(c{=}j, z{=}k) = p(c{=}j)p(z{=}k)$. To find the degree of similarity, we can now apply the Kullback-Leibler divergence between the real distribution and the distribution that assumes independence. In information theory, this corresponds to the mutual information of the random variables C and Z that describe the event of observing classes with documents in the two clusterings [Meil03,HKL+05]:

$$\begin{aligned} I(C,Z) &= D_{\mathrm{KL}}\{p(c,z)\|p(c)p(z)\} \\ &= \sum_{j=1}^{J}\sum_{k=1}^{K} p(c{=}j,z{=}k)[\log_2 p(c{=}j,z{=}k) - \log_2 p(c{=}j)p(z{=}k)] \end{aligned} \tag{92}$$

where the joint probability refers the corpus-wide average co-occurrence of class pairs in documents, $p(c{=}j, z{=}k) = \frac{1}{M}\sum_{m=1}^{M} p(c{=}j|d_m)p(z{=}k|d_m)$.

The mutual information between two random variables becomes 0 for independent variables. Further, $I(C,Z) \le \min\{H(C), H(Z)\}$ where $H(C) = -\sum_{j=1}^{J} p(c{=}j)\log_2 p(c{=}j)$ is the entropy of C. This inequality becomes an equality $I(C,Z){=}H(C){=}H(Z)$ if and only if the two clusterings are equal. Meila used these properties to define the Variation of Information cluster distance measure:

$$D_{\mathrm{VI}}(C,Z) = H(C) + H(Z) - 2I(C,Z) \tag{93}$$

[30] It is immediately clear that this is only as objective as the reference categorisation.

and shows that $D_{\mathrm{VI}}(C, Z)$ is a true metric, i.e., is always non-negative, becomes zero if and only if C=Z, symmetric, and observes the triangle inequality, $D_{\mathrm{VI}}(C, Z)$+$D_{\mathrm{VI}}(Z, X) \geq D_{\mathrm{VI}}(C, X)$[Meil03]. Further, the VI metric only depends on the proportions of cluster assciations with data items, i.e., it is invariant to the absolute numbers of data items.

An application of the VI distance to LDA has been shown in [HKL+05], where the document–topic associations $\underline{\Theta}$ of a corpus of between 20000 news stories are compared to IPTC categories assigned manually to them.

7.3 Test-set likelihood and perplexity

A common criterion of clustering quality that does not require a priori categorisations is the likelihood of held-out data under the trained model, $\log p(\vec{\tilde{w}}_{\tilde{m}}|\mathcal{M})$, i.e., the ability of a model to generalise to the unseen data. These log likelihood values are usually large negative numbers. Therefore, often perplexity is used, originally used in language modelling [AGR03]. Perplexity is defined as the reciprocal geometric mean of the token likelihoods in the test corpus given the model:

$$\mathsf{P}(\tilde{\mathcal{W}}|\mathcal{M}) = \exp -\frac{\sum_{m=1}^{M} \log p(\vec{\tilde{w}}_{\tilde{m}}|\mathcal{M})}{\sum_{m=1}^{M} N_m} \ . \tag{94}$$

This measure can be intuitively interpreted as the expected size of a vocabulary with uniform word distribution that the model would need to generate a token of the test data. A model (or parameter set) that better captures co-occurrences in the data requires fewer possibilities to choose tokens given their document context. Thus lower values of perplexity indicate a lower misrepresentation of the words of the test documents by the trained topics.

The predictive likelihood of a word vector can in principle be calculated by integrating out all parameters from the joint distribution of the word observations in a document. For LDA, the likelihood of a text document of the test corpus $p(\vec{\tilde{w}}_m|\mathcal{M})$ can be directly expressed as a function of the multinomial parameters:

$$p(\vec{\tilde{w}}_{\tilde{m}}|\mathcal{M}) = \prod_{n=1}^{N_{\tilde{m}}} \sum_{k=1}^{K} p(w_n{=}t|z_n{=}k) \cdot p(z_n{=}k|d{=}\tilde{m}) = \prod_{t=1}^{V} \left(\sum_{k=1}^{K} \varphi_{k,t} \cdot \vartheta_{\tilde{m},k} \right)^{n_{\tilde{m}}^{(t)}} \tag{95}$$

$$\log p(\vec{\tilde{w}}_{\tilde{m}}|\mathcal{M}) = \sum_{t=1}^{V} n_{\tilde{m}}^{(t)} \log \left(\sum_{k=1}^{K} \varphi_{k,t} \cdot \vartheta_{\tilde{m},k} \right) \tag{96}$$

where $n_{\tilde{m}}^{(t)}$ is the number of times term t has been observed in document $\tilde{m}$. Note that $\vec{\vartheta}_{\tilde{m}}$ needs to be derived by querying the model, which is done according to Eq. 85. The common method to evaluate perplexity in topic models is to hold out test data from the corpus to be trained and then test the estimated model on the held-out data[31].

Convergence monitoring and training-set measures. As Gibbs sampling shares with all MCMC methods the difficulty to determine when the Markov chain has reached its

[31] This is often enhanced by cross-validation, where mutually exclusive subsets of the corpus are used as hold-out data and the results averaged.

stationary distribution, in practice the convergence of some measure of model quality can be used instead. This extends the use of perplexity and test-set likelihood beyond evaluation of the quality of a converged LDA model towards convergence monitoring.

In addition to using perplexity and likelihood of held-out data for this purpose, in many practical cases it is possible to perform intermediate convergence monitoring steps using the likelihood or perplexity of the training data. Because no additional sampling of held-out data topics has to be performed, this measurement is rather efficient compared to using held-out data. As long as no overfitting occurs, the difference between both types of likelihood remain low, a fact that can even be used to monitor overfitting.

7.4 Retrieval performance

Other standard quality metrics view topic models as information retrieval approaches, which requires that it be possible to rank items for a given query, i.e., an unknown document (see above). The most prominent retrieval measures are precision and recall [BaRi99]. Recall is defined as the ratio between the number of retrieved relevant items to the total number of existing relevant items. Precision is defined as the ratio between the number of relevant items and the total of retrieved items. The goal is to maximise both, but commonly they have antagonistic behaviour, i.e., trying to increase recall will likely reduce precision. To compare different systems, combinations of precision P and recall R metrics have been developed, such as the F_1 measure, $F_1 = 2PR/(P+R)$, which can also be generalised to a weighted F_1 measure, $F_w = (\lambda_P+\lambda_R)PR/(\lambda_P P+\lambda_R R)$. With the given weightings, the preferences to precision or recall can be adjusted. A direct relation between precision and recall to perplexity and language models has been given in [AGR03].

8 Conclusions

We have introduced the basic concepts of probabilistic estimation, such as the ML, MAP and Bayesian inference and have shown their behaviour in the domain of discrete data, especially text. We have further introduced the principle of conjugate distributions as well as the graphical language of Bayesian networks. With these preliminaries, we have reviewed the model of latent Dirichlet allocation (LDA) and a complete derivation of approximate inference via Gibbs sampling, with a discussion of hyperparameter estimation, which mostly is neglected in the literature.

The model of latent Dirichlet allocation can be considered the basic building block of a general framework of probabilistic modeling of text and other discrete data and be used to develop more sophisticated and application-oriented models, such as hierarchical models, models that combine content and relational data (such as social networks) or models that include multimedia features that are modeled in the Gaussian domain. Such a viewpoint has been adopted in the approach of generic topic models in [Hein09].

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