A fully Bayesian view of Latent Dirichlet Allocation

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Abstract

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It is well known that the exponential family of distributions satisfies important stability properties, which lead to elegant, analytical expressions in Bayesian inference, hence its massive use in Bayesian models. One property is that any distribution in that family has a natural conjugate also in that family, and there is a systematic procedure to compute it. For example, the Dirichlet distribution can be derived in this way as a conjugate to the multinomial distribution, and they are both in the exponential family. In the sequel, we are interested in a conjugate to the Dirichlet itself, which is easy to derive by application of the same systematic procedure. We name it here the **Boojum** distribution[1], for lack of a better name. It is a distribution over the positive orthant $\mathbb{R}_+^N$ (the parameter space of the N-dimensional Dirichlet), and has two parameters $m, \boldsymbol{\tau}$ where $m \in \mathbb{R}$ is a scalar and $\boldsymbol{\tau} \in \mathbb{R}^N$ is a vector (as a general rule, the parameter space of the conjugate has dimension one plus the dimension of the parameter space of the original distribution). It is defined, for $\boldsymbol{x} \in \mathbb{R}_+^N$ by

$$\textbf{Boojum}(\boldsymbol{x}; m, \boldsymbol{\tau}) \triangleq \frac{1}{Z(m, \boldsymbol{\tau})} \mathcal{B}(\boldsymbol{x})^m \exp -\boldsymbol{\tau}\boldsymbol{x} \quad (1)$$

where $\mathcal{B}$ denotes the multivariate beta function $\mathcal{B}(\boldsymbol{x}) \triangleq \frac{\prod_n \Gamma(x_n)}{\Gamma(\sum_n x_n)}$ which is also the normalising constant of the Dirichlet distribution with parameter $\boldsymbol{x}$, and $Z(m, \boldsymbol{\tau})$ is the normalising constant of the **Boojum** distribution itself, defined by

$$Z(m, \boldsymbol{\tau}) \triangleq \int_{\boldsymbol{x} \in \mathbb{R}_+^N} \mathcal{B}(\boldsymbol{x})^m \exp -\boldsymbol{\tau}\boldsymbol{x} \, \mathbf{d}\boldsymbol{x}$$

The expression $\boldsymbol{\tau}\boldsymbol{x}$ in the definition denotes the scalar product of the two vectors. Of course, for the distribution to be proper, the normalising constant must be finite, which is not always the case. Although no analytical formula is known for $Z(m, \boldsymbol{\tau})$, one exists for its finiteness:

Proposition 1. *The distribution* $\textbf{Boojum}(m, \boldsymbol{\tau})$ *is proper, i.e.* $Z(m, \boldsymbol{\tau}) < \infty$*, if and only if*[2]

$$\begin{array}{l} \forall n \in N \; \tau_n > 0 \quad \textit{and} \quad m < 1 \quad \textit{and} \\ (m \geq 0 \quad \textit{or} \quad \sum_{n \in N} \exp -\frac{\tau_n}{|m|} < 1) \end{array}$$

Now, conjugacy with the Dirichlet distribution is expressed by the following property.

Proposition 2. *Let* $(\boldsymbol{y}_p)_{p \in P}$ *be a family of random variables over the simplex of* $\mathbb{R}_+^N$*, which are mutually independent given a random variable* $\boldsymbol{x}$ *over* $\mathbb{R}_+^N$*. We have*

$$\begin{array}{ll} \textit{Prior:} & \boldsymbol{x} \sim \textbf{Boojum}(m, \boldsymbol{\tau}) \\ \textit{Observation:} & \forall p \in P \; \boldsymbol{y}_p | \boldsymbol{x} \sim \textbf{Dirichlet}(\boldsymbol{x}) \\ \implies \textit{Posterior:} & \boldsymbol{x} | (\boldsymbol{y}_p)_{p \in P} \sim \textbf{Boojum}(m', \boldsymbol{\tau}') \end{array}$$

where $m' = m - |P| \;\; \boldsymbol{\tau}' = \boldsymbol{\tau} - \sum_{p \in P} \log \boldsymbol{y}_p$

This holds whenever the prior is proper, in which case so is the posterior.

[1] a.k.a. the Snark distribution, because the Snark is a Boojum, you see.

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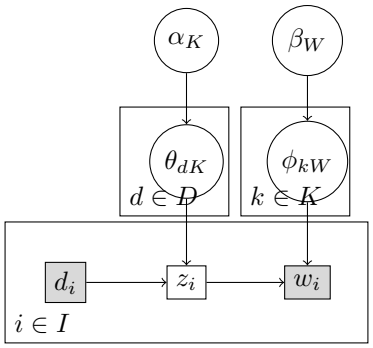
[2] For any whole number N, we use the shorthand $n \in N$ to mean $n \in \{1 \dots N\}$



$$
\begin{aligned}
&p(\alpha_K \beta_W \theta_{DK} \phi_{KW} z_I w_I | d_I) = \\
&\quad p(\alpha_K) p(\beta_W) \\
&\quad \textstyle\prod_{d \in D} p(\theta_{dK} | \alpha_K) \prod_{k \in K} p(\theta_{kW} | \beta_W) \\
&\quad \textstyle\prod_{i \in I} p(z_i | d_i \theta_{DK}) p(w_i | z_i \phi_{KW})
\end{aligned}
$$

$$
\begin{array}{rrcl}
\alpha_K & \sim & p^{(K)} \quad \beta_W & \sim \quad p^{(W)} \\
\forall d \in D & & \theta_{dK} | \alpha_K & \sim \quad \mathbf{Dirichlet}(\alpha_K) \\
\forall k \in K & & \phi_{kW} | \beta_W & \sim \quad \mathbf{Dirichlet}(\beta_W) \\
\forall i \in I & & z_i | d_i \theta_{DK} & \sim \quad \mathbf{Cat}(\theta_{d_i K}) \\
\forall i \in I & & w_i | z_i \phi_{KW} & \sim \quad \mathbf{Cat}(\phi_{z_i W})
\end{array}
$$

$$
\begin{aligned}
\log p(\alpha_K \beta_W \theta_{DK} \phi_{KW} z_I | w_I d_I) &= \log p^{(K)}(\alpha_K) + \log p^{(W)}(\beta_W) - D \log \mathcal{B}(\alpha_K) - K \log \mathcal{B}(\beta_W) \\
&+ \sum_{dk} (\alpha_k - 1) \log \theta_{dk} + \sum_{kw} (\beta_w - 1) \log \phi_{kw} + \sum_{ik} \mathbb{I}[z_i = k] (\log \theta_{d_i k} + \log \phi_{k w_i})
\end{aligned} \tag{2}
$$

Figure 1: The full Bayesian network of the LDA model and the decomposition of its joint distribution q.

4 The LDA model revisited

Given a number D of documents, W of words (or terms), K of topics and I of occurrences, a realisation consists of the following random variables[3]: (i) a tuple $(d_i, z_i, w_i)_{i \in I}$, where for each $i \in I$, the discrete objects $d_i \in D, z_i \in K, w_i \in W$ denote, respectively, the document, the topic and the word associated with occurrence i; (ii) two stochastic matrices θ_{DK} (of dimension $D \times K$) and ϕ_{KW} (of dimension $K \times W$) which characterise each document d as the distribution of topics θ_{dK} and each topic k as the distribution of words ϕ_{kW}; (iii) two positive vectors α_K and β_W which characterise the topics and words of the whole collection.

The space of realisations is that of complete collections of documents: this explains why the collection-level variables α_K and β_W are random, and not parameters. Besides the known size parameters D, W, K, I, the model has two possibly unknown parameters $p^{(K)}$ and $p^{(W)}$, which are distributions for α_K and β_W, respectively. For the sake of symmetry, the occurrence-document vector d_I is considered a random variable, but it is assumed always observed and independent of all the rest, so it could as well have been treated as a known parameter. All probability expressions are conditioned upon it. The full graphical representation of the LDA model is given in Figure 1. Conditioned to the observation of the occurrence-word vector w_I, the log probability is given, up to some additive constant depending only on d_I, w_I, by (2).

[3]In the sequel, we take the convention of not distinguishing the vectors by typesetting them in boldface, but rather by systematically recalling their index ranges as subscripts.

Note that, at this point, we make no assumption on the distributions $p^{(K)}$ and $p^{(W)}$. Our main contribution is precisely in studying the impact of the choice of these distributions. We show that an appropriate choice leads to a new formulation of the variational approximation of LDA, which we investigate.

5 Variational Bayes with Conjugate priors for LDA

The posterior probability given by (2) does not admit an analytical expression. The VB method tries to approximate it, by projecting it onto a simpler space $\mathcal{C}$ of probability distributions, namely that of distributions q of the form

$$
\begin{aligned}
&q(\alpha_K \beta_W \theta_{DK} \phi_{KW} z_I) = q^{(K)}(\alpha_K) q^{(W)}(\beta_W) \\
&\textstyle\prod_{d \in D} q_d(\theta_{dK}) \prod_{k \in K} q_k(\phi_{kW}) \prod_{i \in I} q_i(z_i)
\end{aligned} \tag{3}
$$

Hence, in the variational model, the variables $\alpha_K, \beta_W, \{\theta_{dK}\}_{d \in D}, \{\phi_{kW}\}_{k \in K}, \{z_i\}_{i \in I}$ are assumed independent.

5.1 The VB method

The VB method solves the following optimisation problem:

$$
q^* \quad = \quad \arg\min_{q \in \mathcal{C}} \mathbb{K}(q, \tilde{p}) \quad \text{where} \quad \tilde{p} = p | w_I d_I \tag{4}
$$

Hence q^* is the distribution of class $\mathcal{C}$, i.e. decomposable according to (3), which is closest, for the KL-divergence, to the posterior distribution $\tilde{p}$ given by (2). VB computes an estimate $\dot{q}$ of q^* in $\mathcal{C}$. It proceeds by simple coordinate descent, along the components $\dot{q}_X$, one for each independent variable X in (3). The update, at each step of the coordinate descent focussing

on variable X, is given by

$$\dot{q}_X(x) \quad \leftarrow\propto \quad \exp \mathbb{E}_{y\sim\dot{q}_{\neg X}}[\log \tilde{p}(x,y)] \qquad (5)$$

where the expectation is taken over the set $\neg X$ of all the independent variables in (3) other than X. Hence, the estimate $\dot{q}$ converges to q^*, or at least to a local minimum of $\mathbb{K}(q,\tilde{p})$, taken to be an approximation of $\tilde{p}$. When the right-hand side in (5) does not have an analytical expression, VB uses an additional approximation, by *externally* constraining the estimate $\dot{q}_X$ to be in a specific class of distributions. Typically, one may want to constrain $\dot{q}_X$ to be a Dirac distribution with some parameter $\dot{\pi}_X$ and the update becomes

$$\dot{\pi}_X \quad \leftarrow \quad \arg\max_x \mathbb{E}_{y\sim\dot{q}_{\neg X}}[\log \tilde{p}(x,y)] \qquad (6)$$

The right-hand side of (6) is the mode of the right-hand side distribution in (5), since the closest Dirac approximation of any distribution is the Dirac at its mode.

In the case of the LDA model, it is well known that the choice of conjugate priors (for variable θ_{DK} and ϕ_{KW}) lead to update rules (5) which *naturally* constrain the variational distributions to the following forms[4]:

$$\begin{array}{ll} \forall d \in D & \dot{q}_d(\theta_K) = \mathbf{Dirichlet}(\theta_K; \dot{\alpha}_{dK}) \\ \forall k \in K & \dot{q}_k(\phi_W) = \mathbf{Dirichlet}(\phi_W; \dot{\beta}_{kW}) \end{array}$$

Furthermore, $\dot{q}_i$ is by construction a categorical distribution, with some parameter μ_{iK}. However, the resulting updates do not differentiate between the distributions $\dot{q}_i$ where d_i, w_i are identical, i.e. multiple occurrences of the same word in the same document. Hence, the variational parameter μ_{IK} can be replaced by a parameter μ_{DWK} such that $\mu_{iK} = \mu_{d_i w_i K}$ for all $i \in I$. Likewise, the observation d_I, w_I can be summarised by the sufficient statistics n_{DW}, which is the document-word count matrix:

$$n_{dw} \quad \triangleq \quad |\{i \in I | d_i = d, w_i = w\}|$$

Finally, the updates given by (5) applied to the LDA model are summarised in Figure 2, where the different updates are given labels (in brackets under the arrow) for reference purpose. For clarity sake, we have introduced the intermediate variational quantities $\bar{\alpha}_{DK}$ and $\bar{\beta}_{KW}$ defined by

$$\bar{\alpha}_{dk} \triangleq \mathbb{E}_{\theta_K\sim\dot{q}_d}[-\log\theta_k] \quad \bar{\beta}_{kw} \triangleq \mathbb{E}_{\phi_W\sim\dot{q}_k}[-\log\phi_w]$$

which have a simple analytical expression. One recognises in Figure 2 the standard updates of the LDA model, except maybe for the bottom two **[d]** and **[w]**, discussed below.

[4]To avoid the multiplication of Greek letters, we denote the variational parameters with the same letter as the corresponding model variables, decorated with a dot.

5.2 Treatment of the parameters $q^{(K)}$ and $q^{(W)}$

Let's first justify the update **[d]** of $\dot{q}^{(K)}$ (the same applies to update **[w]** of $\dot{q}^{(W)}$). By eliminating from (2) all the terms which do not involve α_K, hence contribute only a multiplicative constant, and taking expectations on the others, Equation (5) becomes

$$\begin{array}{rcl} \dot{q}^{(K)}(\alpha_K) & \leftarrow\propto & \exp\log p^{(K)}(\alpha_K) - D\log\mathcal{B}(\alpha_K) \\ & + & \sum_d \mathbb{E}_{\theta_{dK}\sim\dot{q}_d}[\sum_k \alpha_k \log\theta_{dk}] \\ & = & p^{(K)}(\alpha_K)\mathcal{B}(\alpha_K)^{-D}\exp\sum_{dk} -\alpha_k\bar{\alpha}_{dk} \\ & \propto & p^{(K)}(\alpha_K)\mathbf{Boojum}(\alpha_K; -D, \sum_d \bar{\alpha}_{dK}) \end{array}$$

where **Boojum** is the conjugate distribution of the Dirichlet in the exponential family introduced in Section 3. To proceed further, we need to choose the parameters $p^{(K)}, p^{(W)}$ (the model priors) so as to make the updates of $\dot{q}^{(K)}, \dot{q}^{(W)}$ concrete. Since the two variables α_K and β_W are parameters of Dirichlet distributions, on θ_{DK} and ϕ_{KW} respectively, we naturally choose their modelling distributions $p^{(K)}, p^{(W)}$ in the conjugate class of Dirichlet, namely **Boojum**. This *naturally* ensures that the corresponding variational distributions $\dot{q}^{(K)}, \dot{q}^{(W)}$ are also in that class.

We first show that the so called EM type 2 hyperparameter estimation, which has been proposed for VB LDA, is in fact a special case of this approach. Indeed, EM in general is known to be a special case of VB, and what we give here is just the pure VB presentation of the method, leading to the same updates. In VB, the method amounts to choosing an "uninformative" $p^{(K)}$, i.e. $p^{(K)} \propto 1$, which is also the improper distribution $\mathbf{Boojum}(0,0)$. Reporting in **[d]**, this *naturally* constrains the distribution $\dot{q}^{(K)}$ to be equal to $\mathbf{Boojum}(-D, \sum_d \bar{\alpha}_{dK})$. However, update **[D]** requires the computation of its expectation, which is intractable. Instead, $\dot{q}^{(K)}$ is *externally* constrained to be a Dirac distribution, hence we can apply Equation (6):

$$\begin{array}{rcl} p^{(K)} \propto 1 & & \dot{q}^{(K)} = \mathbf{Dirac}(\dot{\eta}_K) \\ \dot{\alpha}_{dk} & \leftarrow & \dot{\eta}_k + \sum_w n_{dw}\mu_{dwk} \\ \dot{\eta}_K & \leftarrow & \arg\max \mathbf{Boojum}(-D, \sum_d \bar{\alpha}_{dK}) \end{array}$$

The arg max expression above, computing the mode of the **Boojum** distribution, can be simplified by introducing function $\mathbf{\Phi}$ defined for any vector u_N by

$$\mathbf{\Phi}(u_N) \quad \triangleq \quad \arg\min_{x_N} \log\mathcal{B}(x_N) + u_N x_N$$

The resulting update rules **[D]** and **[d]** are given in Figure 3. By constraining $\dot{q}^{(K)}$ to be Dirac, the computation of its expectation becomes trivial in update **[D]**,

$$\mu_{dwk} \underset{[\mathbf{K}]}{\leftarrow\propto} \exp -(\bar{\alpha}_{dk} + \bar{\beta}_{kw})$$

$$\begin{array}{llll} \bar{\alpha}_{dk} & \leftarrow & \Psi(\sum_{k'} \dot{\alpha}_{dk'}) - \Psi(\dot{\alpha}_{dk}) & \bar{\beta}_{kw} \leftarrow \Psi(\sum_{w'} \dot{\beta}_{kw'}) - \Psi(\dot{\beta}_{kw}) \\ \dot{\alpha}_{dk} & \underset{[\mathbf{D}]}{\leftarrow} & \mathbb{E}[\dot{q}^{(K)}]_k + \sum_w n_{dw}\mu_{dwk} & \dot{\beta}_{kw} \underset{[\mathbf{W}]}{\leftarrow} \mathbb{E}[\dot{q}^{(W)}]_w + \sum_d n_{dw}\mu_{dwk} \\ \dot{q}^{(K)} & \underset{[\mathbf{d}]}{\leftarrow\propto} & p^{(K)}\mathbf{Boojum}(-D, \sum_d \bar{\alpha}_{dK}) & \dot{q}^{(W)} \underset{[\mathbf{w}]}{\leftarrow\propto} p^{(W)}\mathbf{Boojum}(-K, \sum_k \bar{\beta}_{kW}) \end{array}$$

Figure 2: Generic variational updates for the LDA model.

$$\begin{array}{llll} \dot{\alpha}_{dk} & \underset{[\mathbf{D}]}{\leftarrow} & \dot{\eta}_k + \sum_w n_{dw}\mu_{dwk} & \dot{\beta}_{kw} \underset{[\mathbf{W}]}{\leftarrow} \dot{\zeta}_w^{-1} + \sum_d n_{dw}\mu_{dwk} \\ \dot{\eta}_K & \underset{[\mathbf{d}]}{\leftarrow} & \mathbf{\Phi}(\frac{1}{D}\sum_d \bar{\alpha}_{dK}) & \dot{\zeta}_w \underset{[\mathbf{w}]}{\leftarrow} \zeta_w + \sum_k \bar{\beta}_{kw} \end{array}$$

Figure 3: Updates **[D]**, **[W]**, **[d]**, **[w]** in our variants: one is equivalent to the EM type 2 estimation method and the other is original; for the sake of presentation, we apply the former to the document-topic side and the latter to the topic-word side, but they are interchangeable, or the same variant could be applied to both sides.

but at the price of its own update **[d]**, which now requires the computation of the mode of the approximated distribution. In other words, we have traded a complex integration for a complex optimisation, but the latter is still more tractable than the former.

Let's now detail an alternative approach, on the topic-word side for the sake of presentation (but it works just as well on the document-topic side). We still choose $p^{(W)}$ in the **Boojum** class as before, but we don't force its parameter (m, ζ_W) to be 0 as above. Hence, $\dot{q}^{(W)}$ is also in the same class, and let $(\dot{m}, \dot{\zeta}_W)$ be its parameter. The updates are then completely straightforward to derive. The key observation here is that parameter $\dot{m}$ is assigned the expression $m - K$, which never changes in subsequent updates. Furthermore, if we choose $m = K$, that expression is null, i.e. $\dot{m} = 0$. This is particularly helpful, because, then, the intractable $\mathbf{Boojum}(\dot{m}, \dot{\zeta}_W)$ distribution becomes a simple Exponential distribution[5] with rate $\dot{\zeta}_W$, the expectation of which is trivial to compute.

$$\begin{array}{rcl} p^{(W)} = \mathbf{Boojum}(K, \zeta_W) \;\; \dot{q}^{(W)} = \mathbf{Expon}(\dot{\zeta}_W) & & \\ \dot{\beta}_{kw} & \leftarrow & \dot{\zeta}_w^{-1} + \sum_d n_{dw}\mu_{dwk} \\ \dot{\zeta}_w & \leftarrow & \zeta_w + \sum_k \bar{\beta}_{kw} \end{array}$$

The resulting update rules **[W]** and **[w]** are given in Figure 3. Note that parameter ζ_W is still free: it could be set to 0, or preferably to some small machine value (the same for all components) to avoid numerical instability in the inversion of the rate in the expectation of the Exponential in rule **[W]**.

In both variants of LDA, the priors are improper: in the EM type 2 estimation, because it is "uniform" on a space of infinite measure (the positive orthant), and in our case by Proposition 1, since K is obviously not less than 1. None of them is null anywhere on the positive orthant, so the support is preserved.

Using an improper prior is not a problem so long as the posterior is guaranteed to remain proper. While we cannot check that on the true posterior, we can at least check that its approximation computed by the VB method is proper. $\dot{q}^{(W)}$ is an Exponential, and obviously proper: it is easy to show that its parameter $\dot{\zeta}^{(W)}$ always remain strictly within the positive orthant. As for $\dot{q}^{(K)}$, which is a Dirac, we should rather consider the distribution which it approximates, namely $\mathbf{Boojum}(-D, \sum_d \bar{\alpha}_{dK})$, and show that the latter is proper. By Proposition 1, and after a few transformations (essentially replacing $\bar{\alpha}_{DK}$ by its definition in terms of $\dot{\alpha}_{DK}$) we have to show

$$\log \sum_k \exp \frac{1}{D} \sum_d \Psi(\dot{\alpha}_{dk}) < \frac{1}{D} \sum_d \Psi(\sum_k \dot{\alpha}_{dk})$$

And indeed, this is a direct consequence of the convexity of $\log \sum \exp$, together with some known property of function Ψ.

The prior $p^{(W)}$ on β_W is very different in shape from $p^{(K)}$ on α_K. While the latter has a uniform (improper) density, the former is strongly peaked at 0 and sharply decreasing away from it. It tends to favour values of β_W close to 0. But β_W is the parameter of the Dirichlet for ϕ_{kW}, and a Dirichlet with parameter close to 0 tends to favour values towards the borders, and even more the corners, of the simplex. Since ϕ_{kW} is the distribution of words of topic k, being close to the borders and corners of the simplex essentially means being sparse. Hence, our choice of prior favours sparsity in the topic word profiles (the same applies to the

[5] We mean here a multivariate Exponential, product of independent scalar Exponentials.

document topic profile if we choose our prior on that side).

6 Experiments

7 Discussion

Acknowledgements

Use unnumbered third level headings for the acknowledgements. All acknowledgements go at the end of the paper. Be sure to omit any identifying information in the initial double-blind submission!

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