Admixture models and coordinate ascent variational inference

In this lecture we will derive a coordinate ascent variational inference (CAVI) algorithm to do approximate posterior inference in an admixture model.

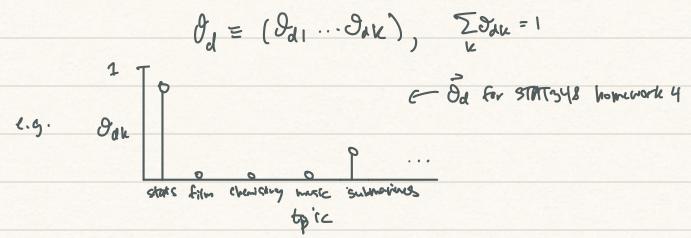
More specifically, the model will be latent Dirichlet allocation (LDA), the most well-known form of admixture model introduced independently by Pritchard, Stephens, Donnelly (2000) for statistical genetics and Blei, Ng, Jordan (2003) for topic modeling.

Admixture model

The data consist of "documents", or more generally groups of data points. For "document" d=1....D:

Each document is a group of Nd "word tokens", or more generally categorical data points. Each token i in document d is:

We assume that each document can be described by a mixture of K topics:



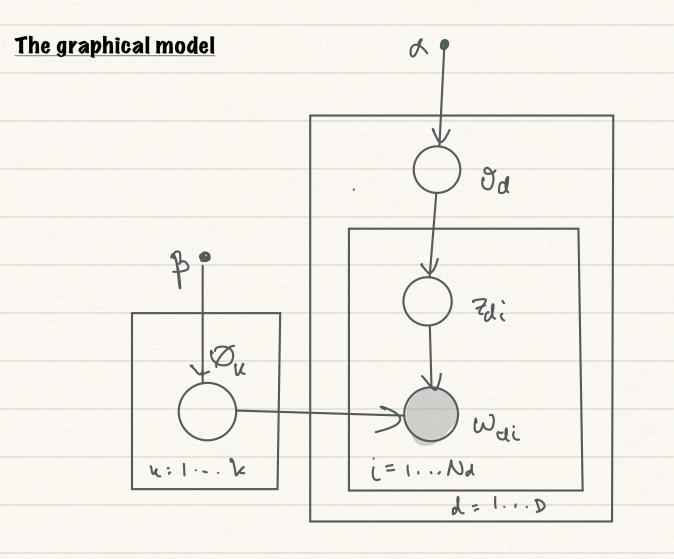
Each "topic" is then defined by a distribution over the vocabulary:

$$\nabla_{\mathbf{k}} = (\nabla_{\mathbf{k}} \cdot \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \cdot)$$
, $\nabla_{\mathbf{k}} \nabla_{\mathbf{k}} \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \nabla_{\mathbf{k}} \cdot \cdot \nabla_{\mathbf{k}} \cdot \nabla_{\mathbf{k$

The generative process is as follows. We assume each word token was drawn from some topic:

Each document is modeled by a mixture model, with mixture weights theta_d, but the whole corpus of documents is then said to be modeled by an admixture model or mixed-membership mixture model.

To complete a Bayesian specification of the model, we place priors over the parameters:



Applications of LDA

- Topic modeling: the data is a corpus of text documents. The goal is to infer a description of the thematic structure of the corpus via the topics.
- Population genetics: each "document" is an individual. At each genetic locus, they can have 0, 1 or 2 mutations. We assume that an individual's genome can be described as an admixture over K ancestral populations ("topics").
- Inference of cell types: each cell has been profiled and is associated with a
 collection of "reads", where each read corresponds to a genetic locus that
 has been expressed. We assume that cells can be described as a mixture over
 cell archetypes, each of which is a distribution over genes.
- Radioactive material detection: each document is a censor, which is a
 collection of "reads" of different levels of rays. We assume each censor
 corresponds to a mixture over topics of rays, each of which corresponds to a
 different kind of material.

Complete conditionals, sufficient stats, "bag of words"

$$\rho(\overline{z}_{di} = k \mid w_{di} : \gamma, -) \quad d \quad \rho(\overline{z}_{di} = k \mid \overline{z}_{d}) \quad \rho(\omega_{di} = \gamma \mid \overline{z}_{di} = k, \overline{D})$$

$$= \frac{\overline{z}_{dk} \not p_{kk} \nu}{\overline{z}_{dij} \not p_{j} \nu}$$

$$\rho(\overline{z}_{d} \mid -) \quad \rho(\overline{z}_{d} \mid d) \quad \overline{\prod} \quad \overline{\prod} \quad \rho(\overline{z}_{di} = k \mid \overline{z}_{d})$$

$$\frac{1}{\overline{z}_{di} = k}$$

$$\frac{1}{$$

$$P(\emptyset_{\mathcal{U}} | -) \neq Dir(\mathcal{B}_{\mathcal{U}}, \mathcal{P}) \xrightarrow{\Pi \Pi} \underset{\gamma}{\Pi} \neq \underset{\mathcal{U}}{\mathbb{Z}_{\mathcal{U}}} = \mathcal{U}) 2(\omega_{\mathcal{U}} = \mathcal{V})$$

$$= Dir(\mathcal{B}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}) \xrightarrow{\mathcal{U}} \underset{\mathcal{U}}{\mathbb{Z}_{\mathcal{U}}} = \mathcal{U}) 2(\omega_{\mathcal{U}} = \mathcal{V})$$

$$= Dir(\mathcal{B}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}) \xrightarrow{\mathcal{U}} \underset{\mathcal{U}}{\mathcal{U}} = \mathcal{U}) 2(\omega_{\mathcal{U}} = \mathcal{V})$$

$$= \sum_{\mathcal{U}} (\mathcal{B}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}})$$

$$= \sum_{\mathcal{U}} 2(\mathcal{B}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}})$$

$$= \sum_{\mathcal{U}} 2(\mathcal{B}_{\mathcal{U}}, \mathcal{P}_{\mathcal{U}}, \mathcal{P}_$$

Notice that the sufficient statistics for the Dirichlet vectors are just the counts of indicators Z. These counts form two matrices:

Consider how we might sample the Z's in a Gibbs sampler, and then compute these statistics:

for
$$d=1...D$$
:

for $\gamma=1...V$:

for $i=1...N_d$:

if $wai=\gamma$:

$$Zai \sim Cat(P_{av})$$

Where $Pav=(Pav) \sim Pavk$, $Pavk=\frac{\partial_{av}\partial_{av}}{\sum \partial_{aj}\partial_{jv}}$

The inner loop over the vocabulary v = 1...V is just a way to show that all indicators z_d for tokens $w_d = v$ are iid from the same complete conditional, described by the probability vector $v_d = v$.

The number of tokens in document d that take value v are:

$$y_{dv} = \sum_{i=1}^{Na} 1(w_{di} = v)$$

Therefore, equivalently, we can sample the sums of indicators from a multinomial.

for
$$d=1...$$

for $v=1...$

$$(y_{dv_1}...y_{dv_k}) \sim Multinoon_{\overline{a}} (y_{dv_k}, P_{dv_k})$$

where $y = \sum_i 1(\omega_{di} = v_i) 1(\overline{z}_{di} = v_i)$

"The number of tokens in document d of word type v assigned to topic k"

The sufficient statistics for the parameters are then just contractions of this 3-dimensional array:

What have we learned? To fit LDA to a corpus of word tokens, we only need the document-word counts:

In other words, the generative process encodes the "bag of words" assumption. The order or the unique identity of the different word tokens does not matter. All that matters is how many tokens of each word type v are in each document d: y_dv .

This is a **very** bad assumption about how text is actually generated. Nevertheless, when applied to documents, LPA learns interpretable latent structure that can be useful at a high level.

CAVI for LDA

We will make the simplifying "mean-field assumption" that the q-distribution is a factorized family. This will facilitate the optimization problem:

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Recall from last time the ELBO objective function we will seek to maximize:

argmin
$$kL(q(...) | p(...|w) = argmax = \left[log \frac{p(...)}{q(...)}\right]$$

$$= ELBO(q)$$

Since q factorizes, it will be convenient to maximize the ELBO coordinate-wise (i.e., updating each factor, holding all other factors fixed).

e.g.
$$q^*(\partial_d) = \underset{q(\partial_d)}{\operatorname{argmax}} E(BO(q)$$

For any factor, the optimal update takes the following form, using theta_d as an example:

where the expectation is with respect to all factors in q except the given one, and the term inside is the complete conditional of the given variable under the true model.

This general form for the optimal update is given by Bishop (2006). Let's confirm that it is true. Consider the KL from any other setting of the density q(theta_d) to the (supposedly) optimal one:

$$KL(q(\theta_d) || q''(\theta_d)) = \underbrace{\mathbb{E}_{q(\theta_d)} \left[\log q(\theta_d) - \log q''(\theta_d) \right]}_{q(\theta_d)} \left[\log q(\theta_d) \right] - \underbrace{\mathbb{E}_{q(\theta_d)} \left[\log p(\theta_d) - \log q''(\theta_d) \right]}_{d}$$

$$d - H(q(\theta_d)) - \underbrace{\mathbb{E}_{q} \left[\log p(\theta_d), 7 \mid W \right]}_{d}$$

$$d - ELBO(q)$$

So indeed to maximize the ELBO wrt q(theta_d) you minimize the KL to the stated optimal update.

As we've seen before with EM, the optimal update takes the form of a geometric mean. This means that if the complete conditional is an exponential family, the optimal update to the factor is also a member of that same exponential family:

where the complete conditional's natural parameter is potentially a function of data and other latent variables.

then
$$q^{*}(\vartheta_{d}) = f(\vartheta_{d}; \mathbb{E}[\eta_{d}(\cdots)])$$

where the natural parameter of this factor is the expectation under the variational distribution (not including this factor) of the complete conditional's natural parameter.

To be clear, this says two things: 1) that the optimal factor is in the same exponential family as the complete conditional, and 2) that its natural parameter takes the form above. To be explicit about this we will introduce notation for the variational parameters (which until now have been implicit):

$$\begin{array}{cccc}
\boxed{0} & q^*(\partial_d) &= q(\partial_d; \vec{\eta}_d) &= f(\partial_d; \vec{\eta}_d) \\
\boxed{0} & \vec{\eta}_d &= \mathbb{E}_{q} \left[\gamma_d(\cdots) \right]
\end{array}$$

we are using a tilde to distinguish the **variational parameter** from the parameter of the complete conditional in the true model.

In the case, the complete conditional is Dirichlet. The natural parameter of the Dirichlet is just its shape parameters (the usual parameters), so:

Let's take a look at the expectations:

$$E_{q} \left(Y_{dk} \right) = E_{q} \left(\sum_{i \neq j} 1(z_{id} - k) \right)$$

$$= \sum_{i \neq j} q(z_{id} - k)$$

So we see that this depends on the factors q(z_id).

The normalizer of the probability does not depend on k (the assumed value of z_id:

Here we are introducing new notation for the geometric expected value.

Putting it altogether:

Do we know these geometric expected values? In this case, the relevant q-distribution is a Dirichlet (as we showed in the last derivation). Both the arithmetic and geometric expected values under a Dirichlet are known in closed form:

$$(X_{1}...X_{K}) \sim Dir(d_{1}...d_{K})$$

$$E[X_{k}] = \frac{d_{k}}{\sum d_{i}}, \quad C(X_{k}) = \frac{exp(\psi(d_{k}))}{\sum exp(\psi(d_{i}))}$$
where $\psi(\cdot)$ is digenoral function

CAVI for LDA:

Computing the ELBO:

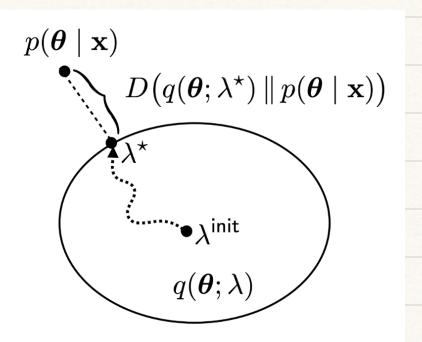
$$\begin{aligned}
& = \underbrace{\mathbb{E}_{q} \left[\log_{p} \frac{P(0, 0.7, w)}{q(0, 0.7, w)} \right]}_{q(0, 0.7, 0.7)} + \underbrace{\mathbb{E}_{q} \left[\log_{p} \frac{P(0, 0.7, 0.7)}{q(0, 0.7, 0.7)} \right]}_{q(0, 0.7, 0.7)} \\
& = \underbrace{\mathbb{E}_{q} \left[\log_{p} P(w | - 1) \right] + \mathbb{E}_{q} \left[\log_{p} \frac{P(0)}{q(0)} \cdot \frac{P(0)}{q(0)} \cdot \frac{P(0)}{q(0)} \cdot \frac{P(0)}{q(0)} \right]}_{q(0, 0.7, 0.7)}
\end{aligned}$$

$$\begin{aligned}
E_{q} \left[\log \frac{p(0)}{q(0)} \right] &= \sum_{d} \left[E_{q} \left[\log \frac{p(0d)}{q(0d)} \right] \right] \\
&= -\sum_{d} \left[E_{q} \left(Q_{q} \right) \right] \left[p(0d) \right] \\
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&= -\sum_{d} \left[E_{q} \left(Q_{q} \right) \right] \\
&= -\sum_{d}$$

The KL between two Dirichlets is known in closed form. The other terms can be simplified in similar ways and will end up involving simple expectations under the variational distribution.

What is CAVI doing?

Popping up a level, CAVI is finding the member of a simple parametric family that is closest in KL to the exact posterior. It does so by maximizing the ELBO coordinate-wise. Here's the picture:



In this case, theta represents all latent variables parameters, x is the data, and lambda are the variational parameters. Lambda* represents the value of the variational parameters that brings q(...) closest in KL to the exact posterior. Since q is a factorized family though, there may always be a gap.

Stochastic variational inference (SVI)

For very large data sets, even CAVI can be too slow to run. In this setting, when the model has exponential family complete conditionals we can turn a CAVI algorithm into a scalable stochastic variational inference (SVI) algorithm.

To explain this, we will move to a much more general description of a model. The notation will be different—e.g., Z in this section will not be the same as Z in the previous sections.

Here's a very general description that many models can be written as:

data : $\times_1 \cdots \times_n$

local latent variables : 2, ... Zn

global latent variables : \sim aka "parameters"

hyperparameters : 🕹

The complete data likelihood for data point i is:

The conjugate prior is:

$$p(\eta | x) = f(\eta | x) \quad \alpha_{\eta} \quad h_{c}(\eta) \exp(x^{T}t_{c}(\eta))$$

$$t_{c}(\eta) = [\eta, -\alpha_{g}(\eta)]^{T}$$

The complete conditional is then:

where the natural parameter of the complete conditional of the parameter is:

$$d_n = \left[d_1 + \sum_{i=1}^n t_i(z_{ii} \times i), d_2 + n\right]^T$$

We will setup a variational distribution that factorizes:

$$q(2, \eta) = q(\eta; \lambda) \stackrel{\pi}{\pi} q(2; ; \kappa;)$$

where lambda and gamma_i are the variational parameters.

As we saw in the last section, the optimal CAVI update for the factor over eta would be

$$q''(n; \lambda) dn = \exp(\frac{1}{4} [\log p(n|-)])$$

$$dn = h. (n) = \exp(\frac{1}{4} [dn])$$

$$= f(n), = k$$

Although we derived this in another way, we could think about this in terms of gradients of the ELBO (or KL divergence). Consider taking the following gradient with respect to the variational parameter lambda:

Terms not involving lambda or eta will drop. We can also add a constant into the numerator to obtain:

Now assume that q(...) is the same exponential family as the complete conditional

The expectation is over both global and local latents, and the natural parameter of the complete conditional is a function of local latents:

The expectation of the sufficient statistics is the mean parameter of any expfam, equal to the gradient of the log normalizer.

=
$$\nabla^2_{\lambda} \alpha_{c}(\lambda) \left(E_{\rho} \left[\alpha_{n} \right] - \lambda \right) + \nabla_{\lambda} \alpha_{c}(\lambda) - \nabla_{\lambda} \alpha_{c}(\lambda) \right)$$

Hessian
$$\left[\nabla^2_{\lambda} \alpha_{c}(\lambda) \right]_{ij} = \frac{3}{3} \nabla^2_{ij} \alpha_{c}(\lambda)$$

The term out front is then the Hessian of the log-normalizer (matrix of second-order derivatives). It's immediately clear from the gradient that the optimal setting of the variational parameter is:

which we already knew.

Unpacking this expectation, we see that it involves a sum over n data points:

$$\frac{1}{2} \left[\frac{1}{2} \left(\frac{1}{2}$$

If there are many data points, it may be prohibitive to update all the local factors q(zi).

Instead, we will derive an algorithm that sub-samples our data. To do so, we will re-cast variational inference in terms of stochastic optimization.

Consider the following stochastic gradient ascent algorithm

where epsilon_t is the step-size at iteration t and we are following the gradient of an estimate of the ELBO, which might be different at each iteration.

If our estimator of the ELBO is unbiased—i.e.,

and if the sequences of step-sizes follows the Robins-Monroe conditions—i.e.m

then the parameter will eventually converge to a local mode of the ELBO:

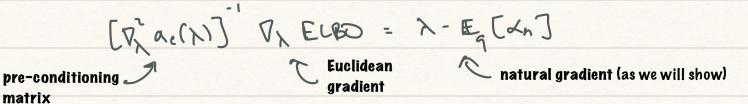
Why does this help us? Because unbiased estimators of gradients can often be derived by sub-sampling the data. Consider a gradient of the following form:

$$\sqrt{\sum_{i=1}^{n} d_i(x_i, t_i, \lambda)}$$

Then we could sub-sample the data points uniformly at random to construct the following unbiased estimator:

Unfortunately the Euclidean gradient of the ELBO does not have this form...

...however the pre-conditioned Euclidean gradient does:



It turns out that pre-conditioning the Euclidean gradient in this particular way (with the inverse of the Hessian) gives us the **natural gradient** when the complete conditionals are all exponential families.

What is a **natural gradient**? Amari (1998) introduced the idea of natural gradient ascent for fitting probabilistic models. The natural gradient is defined by the Euclidean gradient pre-conditioned by the **inverse Fisher information** matrix, which in our setting would be:

where the Fisher information matrix is defined as:

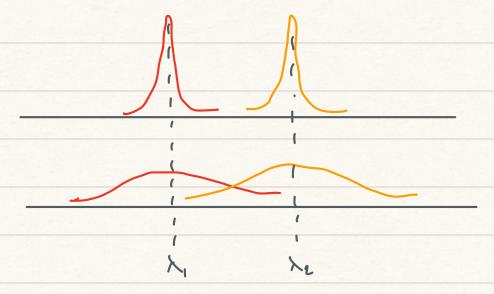
For exponential families, the Fisher information is:

$$= -\nabla_{\Lambda}^{2} \left(\mathbb{E} \left[t(\eta) \right]^{T} \lambda - \alpha(\lambda) \right)$$

$$= \nabla_{\Lambda}^{2} \alpha(\lambda)$$

So the Hessian of the log-normalizer is the Fisher information for exponential families.

The natural gradient is a **local re-scaling** of the Euclidean gradient to account for the fact that distances between probability distributions is not equal to the Euclidean distance between their parameters. Here's a simple example:



In both plots, the Euclidean distance between the parameters of the orange and red distributions is the same. However the KL-divergence between the two distributions is much higher in the top than in the bottom.

Consider then the following natural gradient step:

In our settings, the natural gradient equals:

Re-arranging terms:

Recall that the expectation of the posterior natural parameter equals

$$\mathbb{E}_{q}\left[\lambda_{n}\right] = \mathbb{E}_{q}\left[\lambda_{1} + \sum_{i=1}^{n} t(z_{i}, x_{i})\right] = \left[\lambda_{1} + \sum_{i=q} \left[t(z_{i}, x_{i})\right]\right]$$

So we can replace this expectation with an unbiased estimator of the expectation:

$$\frac{1}{4} \left[\frac{1}{4} + n \, \mathbb{E}_{q} \left[\frac{1}{4} (2:1 \times 1) \right] \right], \quad c \sim \text{Difform} (1...n)$$

Putting it altogether, here is the **stochastic VI** algorithm, which performs stochastic natural gradient ascent via data sub-sampling:

subsample a data point

update the factor for the local latent variable

take a natural gradient step in the global latent variable

