1 Introduction

A central question in many probabilistic clustering problems is how many distinct clusters are present in a particular dataset. A Bayesian nonparametric (BNP) model addresses this question by placing a generative process on cluster assignment, making the number of distinct clusters present amenable to Bayesian inference. However, like all Bayesian approaches, BNP requires the specification of a prior, and this prior may favor a greater or fewer number of distinct clusters. In practice, it is important to quantitatively establish that the prior is not too informative, particularly when—as is often the case in BNP—the particular form of the prior is chosen for mathematical convenience rather than because of a considered subjective belief.

We derive local sensitivity measures for a truncated variational Bayes (VB) approximation based on the Kullback-Leibler (KL) divergence. Local sensitivity measures approximate the nonlinear dependence of a VB optimum on prior parameters using a local Taylor series approximation [Gustafson, 1996, Giordano et al., 2017]. Using a stick-breaking representation of a Dirichlet process, we consider perturbations both to the scalar concentration parameter and to the functional form of the stick-breaking distribution. As far as the authors are aware, ours is the first analysis of the local sensitivity of BNP posteriors when using a VB approximation.

Unlike previous work on local Bayesian sensitivity for BNP [Basu, 2000], we pay special attention to the ability of our sensitivity measures to extrapolate to different priors, rather than treating the sensitivity as a measure of robustness per se. Extrapolation motivates the use of multiplicative perturbations to the functional form of the prior for VB, as the KL divergence is then linear in the perturbation. Additionally, we linearly approximate only the computationally intensive part of inference—the optimization of the global parameters—and retain the nonlinearity of easily computed quantities as functions of the global parameters.

We apply our methods to estimate sensitivity of the expected number of distinct clusters present the Iris dataset [Anderson, 1936, Fisher, 1936] to the BNP prior specification. We evaluate the accuracy of our approximations by comparing to the much more expensive process of re-fitting the model.

2 Model and Inference

Data and model. We use the Iris dataset [Anderson, 1936, Fisher, 1936], which contains 150 observations of three different types of iris flowers. We use measurements of their sepal length, sepal width, petal length, and petal width to cluster the data with the goal of recovering the three species. Let \( y_n \in \mathbb{R}^4 \) be these four measurements for flower \( n \).

In the spirit of BNP, let us suppose that there there are an infinite number of distinct species of iris in the world, indexed by \( k = 1, 2, 3, \ldots \), only some finite number of which are present in our observed dataset. Let \( z_n \) denote the index of the species (i.e. the cluster) to which flower \( n \) belongs, i.e.,
$z_n = k$ for exactly one $k$. Each cluster has mean $\mu_k \in \mathbb{R}^d$ and covariance $\Sigma_k \in \mathbb{R}^{d \times d}$, and we write the collections as $\mu = (\mu_1, \mu_2, \ldots)$ and $\Sigma = (\Sigma_1, \Sigma_2, \ldots)$. Our data-generating process given the model parameters is then

$$y_n | z_n, \mu, \Sigma \sim \mathcal{N}\left(y_n, \sum_{k=1}^{\infty} I\{z_n = k\} \mu_k, \sum_{k=1}^{\infty} I\{z_n = k\} \Sigma_k\right), \quad n = 1, \ldots, N.$$  

For $\mu$ and $\Sigma$, we use dispersed IID conjugate priors. For the prior on the cluster memberships $z_n$, we use a stick breaking representation of a BNP Dirichlet process prior [McCloskey 1965, Ferguson 1973, Patil and Taillie 1977, Sethuraman 1994]. Specifically, we define latent stick lengths $\nu = (\nu_1, \nu_2, \ldots)$, a concentration parameter $\alpha > 0$, and base stick-breaking distribution $p_0 (\nu_k | \alpha) = \text{Beta} \left( \nu_k | 1, \alpha \right)$. The prior on the cluster assignments $z_n$ for $n = 1, \ldots, 150$ is then given by

$$\nu | \alpha \sim \prod_{k=1}^{\infty} p_0 (\nu_k | \alpha), \quad \text{with} \quad \pi_k | \nu := \nu_k \prod_{j=1}^{k-1} (1 - \nu_j) \quad \text{and} \quad z_n | \pi \overset{iid}{\sim} \text{Categorical}(\pi). \quad (1)$$

The concentration parameter $\alpha$ and stick-breaking prior $p_0$ thus determine our prior belief about the number of clusters present. This prior specification and the observed data combine to inform our posterior belief about the posterior number of clusters. We will be examining the sensitivity of our posterior belief to our choice for $\alpha$ and $p_0$.

**Variational approximation.** It is difficult to calculate the posterior $p (\nu, \mu, \Sigma, z | y)$, both because the normalizing constant is intractable and because there are an infinite number of latent clusters in a true BNP representation. In order to perform approximate inference, we use a truncated VB approximation using $K = 30$ clusters [Blei and Jordan 2006], and assert that the later clusters are essentially unoccupied in the posterior. For compactness of notation, let $\theta = (\nu, \mu, \Sigma)$ denote the collection of “global” parameters, i.e., parameters whose values affect the data-generating process of every observation $y_n$. Let $\delta (\cdot)$ denote a delta function. We define a class of approximating distributions for VB as

$$Q := \left\{ q : q (\theta, z) = \left( \prod_{k=1}^{K} q (\nu_k) \delta (\mu_k) \delta (\Sigma_k) \right) \left( \prod_{n=1}^{150} q (z_n) \right) \right\},$$

where $q (\nu_k) = \text{Lognormal} (\nu_k)$ and $q (z_n) = \text{Categorical} (z_n)$.

The family $Q$ is parameterized by a finite-dimensional vector containing the locations of the delta functions and the parameters for the lognormal distributions, which we denote by $\eta_\theta$, and the parameters for the categorical distributions, which we denote by $\eta_z$. We write the combined parameters as $\eta = (\eta_\theta, \eta_z)$. That is, $\eta$ is defined such that $Q = \{ q : q (\theta, z) = q (\theta | \eta_\theta) q (z | \eta_z) \}$. The variational approximation is then given by $\eta^* = \arg \min_\eta KL \left( q (\theta, z | \eta) \| p (\theta, z | y) \right).$

It will be important later to note that it is easy to calculate the optimal $\eta^*_\theta$ for a given $\eta_\theta$ because the model is conditionally conjugate, i.e., $p (z | \theta, y)$ is categorical, and so is $q (z | \eta_z)$. Specifically, there exists an easily-calculated, closed form for $\eta^*_z (\eta_\theta) = \arg \min_{\eta_z} KL \left( q (\theta | \eta_\theta) q (z | \eta_z) \| p (\theta, z | y) \right).$

**Target posterior quantity.** We are interested in the inferred number of clusters present in the observed data. This quantity can be expressed as an expectation with respect to $q (z | \eta_z)$, and therefore as a function of $\eta^*_\theta$ via the relation $\eta^*_z (\eta_\theta)$:

$$g (\eta^*_\theta) := \mathbb{E}_{q (\theta, z | \eta^*_\theta)} [\# \{ \text{distinct clusters} \}] = \mathbb{E}_{q (z | \eta^*_z (\eta^*_\theta))} \left[ \sum_{k=1}^{K} \left( 1 - \prod_{n=1}^{N} I \{ z_n \neq k \} \right) \right]. \quad (2)$$

For a given optimal set of global variational parameters, $g (\eta^*_\theta)$ can be computed with Monte-Carlo draws of the cluster indicators, $z \overset{iid}{\sim} q (z | \eta^*_z (\eta^*_\theta))$. We will denote Monte-Carlo expectations by $\hat{\mathbb{E}} [\cdot]$.  

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1 We use the lognormal distribution rather than the conjugate Beta distribution because the lognormal makes numerical integration easier when re-optimizing using non-conjugate $p_0$. Were one to simply rely on our sensitivity measures and not re-optimize, there would be no need for numerical integration, and the more convenient Beta variational approximation could be used.
3 Hyper-parameter sensitivity

General hyperparameter sensitivity. We wish to approximate the sensitivity of $g(\eta_0^*)$ to perturbations of the value of $\alpha$ and to the functional form of $p_0$. To do this, we will call on a general result for the sensitivity of VB optima to vectors of real-valued hyperparameters. Suppose the exact posterior is parameterized by a real-valued hyperparameter $\epsilon$, i.e., the posterior is given by $p(\theta, z | y, \epsilon)$. In the present work, $\epsilon$ will parameterize perturbations to the prior, as we will describe in more detail shortly. Then the optimal variational approximation is also a function of $\epsilon$ through the minimization of the KL divergence. We can define

$$KL(\eta_0, \epsilon) := KL(q(\theta, z | \eta_0, \eta_0^*(\eta_0)) || p(\theta, z | y, \epsilon))$$

and $\eta_0^*(\epsilon) = \arg\min_{\eta_0} KL(\eta_0, \epsilon).$ (3)

In general, the dependence of $\eta_0^*(\epsilon)$ on $\epsilon$ is complex and nonlinear, but under mild regularity conditions—which are satisfied in the present case—we may approximate it with a first-order Taylor series. Giordano et al. [2017, Theorem 2] gives these conditions as well as a closed form expression for this Taylor series. Without loss of generality, let $\epsilon = 0$ represent the unperturbed posterior, so that $p(\theta, z | y, \epsilon = 0) = p(\theta, z | y)$. Define the Hessian $H := \partial^2 KL(\eta_0, \epsilon) / \partial \eta_0 \partial \eta_0^T |_{\eta_0 = \eta_0^*, \epsilon = 0}$ and $f_\eta := \partial^2 E_{q(\theta, z | \eta_0, \eta_0^*(\eta_0))}[\log p(\theta, z, \epsilon)] / \partial \eta_0 \partial \epsilon^T |_{\eta_0 = \eta_0^*, \epsilon = 0}$. Then

$$\eta_0^*(\epsilon) - \eta_0^*(0) \approx \frac{df_\eta^*(\epsilon)}{d\epsilon} \bigg|_{\epsilon = 0} = -H^{-1} f_\eta \epsilon,$$ (4)

Note that $H$ and $f_\eta$ can be easily evaluated using automatic differentiation without any need to re-optimize for different $\epsilon$ [Maclaurin et al., 2015]. Furthermore, the Hessian $H$ needs to be factorized (e.g. with a Cholesky decomposition) or inverted only once and then re-used to approximate $\eta_0^*(\epsilon)$ for many different perturbations.

Allowing nonlinearity in computationally easy steps. Note that the complete mapping $\epsilon \mapsto \hat{E}_{q(z | \eta_0^*)} [\# \{\text{distinct clusters}\}]$ is, in general, composed of many highly nonlinear steps:

$$\epsilon \mapsto \eta_0^*(\epsilon) \mapsto \eta_0^*(\eta_0^*) \mapsto \text{Draws from } z \sim q(z | \eta_0^*) \mapsto \hat{E}_z [\# \{\text{distinct clusters}\}].$$

However, only the first step, $\epsilon \mapsto \eta_0^*(\epsilon)$, is computationally intensive (re-solving the optimization problem in Equation 3 with a new $\epsilon$), and it is precisely this first step which we approximate linearly using Equation 4, i.e., with $\epsilon \mapsto \eta_0^*(0) - H^{-1} f_\eta \epsilon$. Consequently, our approximations retain the nonlinearity in the mapping $\eta_0^* \mapsto \hat{E}_z [\# \{\text{distinct clusters}\}]$.

Furthermore, we attempt to improve the linearity of the dependence of $\eta_0^*$ on $\epsilon$ by using an unconstrained parameterization for $\eta_0$ as in [Stan Team, 2015] and [Kucukelbir et al., 2015].

Sensitivity to $\alpha$. Let $\alpha_0$ be a base value of $\alpha$ at which we optimize for $\eta^*$. By simply taking $\epsilon = \alpha - \alpha_0$, and

$$f_\eta^\alpha := \frac{\partial^2 E_{q(\theta, z | \eta_0, \eta_0^*(\eta_0))}[\log p(\nu | \alpha)]}{\partial \eta_0 \partial \alpha^T} |_{\eta_0 = \eta_0^*, \alpha = \alpha_0},$$

we can approximate

$$\eta_0^{LIN}(\alpha) := \eta_0^* - H^{-1} f_\eta^\alpha(\alpha - \alpha_0) \approx \eta_0^*(\alpha).$$

We can then approximate $g(\eta_0^*(\alpha)) \approx g(\eta_0^{LIN}(\alpha))$.

On the Iris data, we evaluated the expected number of clusters for a range of $\alpha$ between 0.5 and 15. Then we chose three $\alpha_0$ values, 3, 8, and 13, and constructed the linear approximation centered at each of these values of $\alpha_0$. We note that the linear approximation is more accurate when extrapolating from more clusters to fewer clusters, as can be seen from the fact that the linear approximation in the rightmost panel of Figure 1 is accurate across the entire range of $\alpha$, whereas the leftmost panel is not.
Sensitivity to functional perturbations. In order to measure sensitivity to changing the functional form of the prior on the sticks, we define a parametrized class of multiplicative perturbations to the base density $p_0$ and apply Equation 4. Specifically, fix a multiplicative perturbation $\phi(\cdot) : [0,1] \to (0,\infty)$ (recall that the stick lengths $\nu_k$ lie in $[0,1]$). Fix some $\delta \in [0,1]$. We then define a $\delta$-contaminated prior $p_c$ by

$$p_c(\nu_k | \delta, \phi) := \frac{p_0(\nu_k)\phi(\nu_k)^\delta}{\int_0^1 p_0(\nu')\phi(\nu')^\delta d\nu'},$$

The contaminating prior $p_c$ is defined so that $\delta \in [0,1]$ interpolates multiplicatively between the original prior, $p_0$, and a prior proportional to $\phi(\nu_k)p_0$. For example, we might consider a different prior for the sticks, say $p_1(\nu_k)$. Letting $\phi(\nu_k) = p_1(\nu_k)/p_0(\nu_k)$, we recover $p_0$ at $\delta = 0$ and swap the original prior for the new prior by taking $\delta \to 1$.

For a fixed $\phi$, we can use Equation 4 by taking $\epsilon = \delta$ and

$$f_{\delta,\phi} := \frac{\partial^2 E_q(\theta, z | \eta_\theta,\eta_{z_{\ast}}(\eta_\theta))}{\partial \eta_\theta \partial \delta} \bigg|_{\eta_\theta = \eta_{\ast}, \delta = 0} = \frac{\partial E_q(\theta, z | \eta_\theta,\eta_{z_{\ast}}(\eta_\theta))}{\partial \eta_\theta} \bigg|_{\eta_\theta = \eta_{\ast}} \sum_{k=1}^{K} \log \phi(\nu_k),$$

Because we have used a multiplicative perturbation, $f_{\delta,\phi}$ is linear in $\delta$, which we might expect to improve the fidelity of a linear approximation. Indeed, for the purposes of extrapolating to different priors when using VB based on KL divergence, this fact appears to recommend multiplicative perturbations amongst the class of nonlinear perturbations considered by [Gustafson 1996].

Figure 1: Comparison of the expected number of clusters computed by re-optimizing versus the linear approximation. The blue vertical line indicates the location of $\alpha_0$.

In Figure 2, we show results for the functional perturbation $\phi(\nu_k) = 1 - e^{\nu_k}$. We find that the linear approximation in this case was able to capture the direction of the perturbation, (the expected number of clusters increased under the first perturbation, decreased under the second), although as $\delta \to 1$ the quality of the approximation degraded.

For more experimental results, see Appendix A.
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Appendices

A Further results

We consider a modification to the expected number of posterior clusters defined in Equation 2. We wish to count only the clusters with at least $t$ observations, rather than the total number of distinct clusters. Hence, our posterior target quantity becomes,

$$g_t(\eta^*; \theta) := E_{q(z|\eta^*)} \left[ \# \{ \text{clusters with at least } t \text{ data points} \} \right].$$

Note that $t = 0$ reduces to the original target posterior defined in the equation 2.

Equation 7 defines an in-sample quantity, that is, the expected number of clusters we expect to see in the current Iris dataset. We also consider a posterior predictive quantity, or the number of clusters we expect see in a new dataset of 150 iris flowers, given our posterior knowledge about the stick-breaking process. This is an expectation over the variational distribution of the sticks $\nu$, defined as

$$g_{t, \text{pred}}(\eta^*; \theta) := E_{q(\nu|\eta^*)} \left[ \# \{ \text{clusters in new data set with at least } t \text{ data points} \} \right].$$

where $\pi_k$ are the cluster probabilities induced by the the sticks $\nu$.

Like before, and as described in section 3, only the dependence of $\eta^*$ on the prior perturbation is approximated linearly. Given a $\eta_0^*$ these expectations are computed with Monte-Carlo samples from the variational distribution $q(z|\eta^*_0(\eta^*))$ for the in-sample expectation, $q(\nu|\eta^*_0)$ in the predictive expectation.

Figure 3 shows both the in-sample and predictive expected number of distinct clusters (i.e. $t = 0$). The linear approximation does equally well for both the in-sample and the predictive quantity. It works best when we set $\alpha_0 = 13$, when we approximate from having more clusters to fewer clusters.

Next, figure 4 shows both the in-sample and predicted expected number of clusters with at least three observations ($t = 3$). Again the linear approximation is best when we start at $\alpha_0 = 13$ and extrapolate to fewer clusters.

We next consider functional perturbations to the prior on the sticks. Figure 5 shows the effect of our choice of $\phi$ on the expected number of distinct clusters ($t = 0$). Both the in-sample and the predictive quantities are displayed. The approximation is most accurate at small $\epsilon$, though the predictive quantity for the first perturbation was fairly accurate for the entire range of $\epsilon \in [0, 1]$.

Finally, we consider the same functional perturbation to the stick priors, but with the threshold for counting a cluster at $t = 3$. Figure 5 displays the comparison of the linear approximation against the refitted values, for both the in-sample and the predictive quantities. In this case, the choice of perturbation did not significantly move the number of thresholded clusters in the re-fitted values.
Figure 3: The in-sample expected number of distinct clusters (Top), and the predictive expected number of distinct clusters (Bottom). Comparison of these values computed by re-optimizing versus the linear approximation. The blue vertical line indicates the location of $\alpha_0$.

Figure 4: The in-sample expected number of distinct clusters with at least three observations (Top), and the corresponding predictive quantity (Bottom). Comparison of these values computed by re-optimizing versus the linear approximation. The blue vertical line indicates the location of $\alpha_0$. 
Figure 5: The effect of prior perturbation on the expected number of distinct clusters ($t = 0$). Left column: the original prior $p_0$ in red, the perturbed prior $p_c$ in blue. Middle: linearly approximated vs. re-fitted in-sample expected number of clusters. Right: linearly approximated vs. re-fitted predictive expected number of clusters.

Figure 6: The effect of prior perturbation on the expected number of clusters with at least three data points. ($t = 3$). Left column: the original prior $p_0$ in red, the perturbed prior $p_c$ in blue. Middle: linearly approximated vs. re-fitted in-sample expected number of clusters. Right: linearly approximated vs. re-fitted predictive expected number of clusters.