Bayesian Theory and Computation

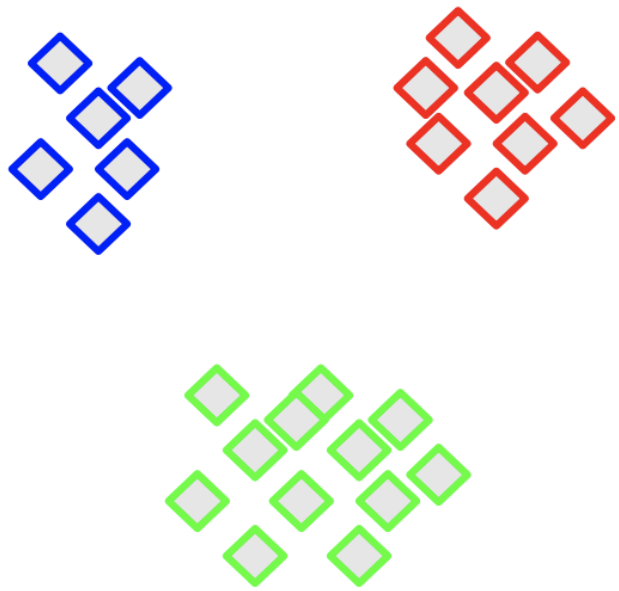
Lecture 18: Dirichlet Processes

Cheng Zhang

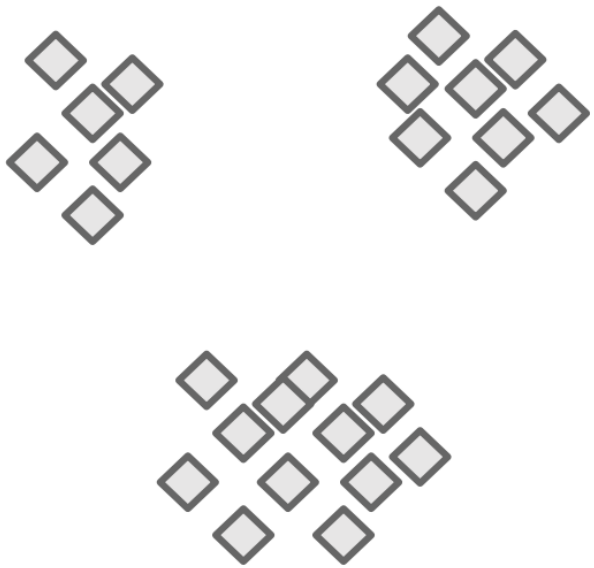
School of Mathematical Sciences, Peking University

May 12, 2025

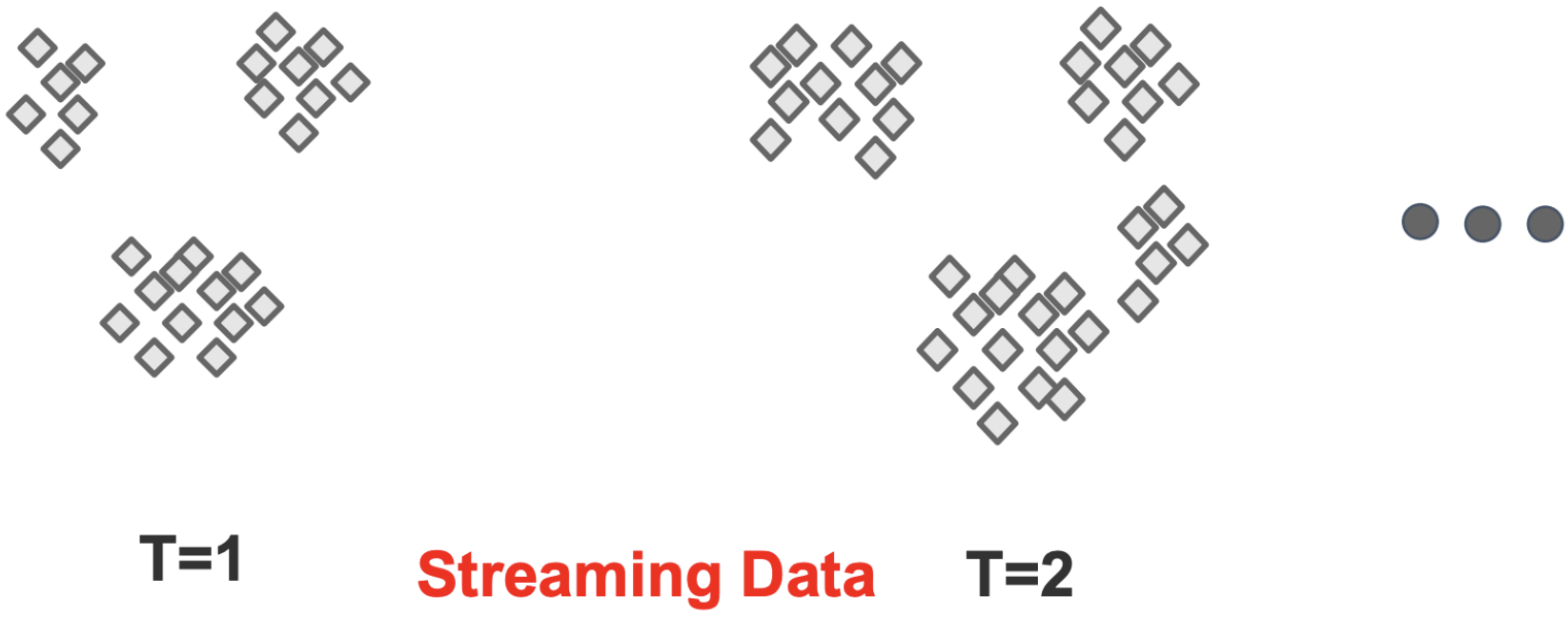
How to choose the number of clusters?



How to choose the number of clusters?



How to choose the number of clusters?



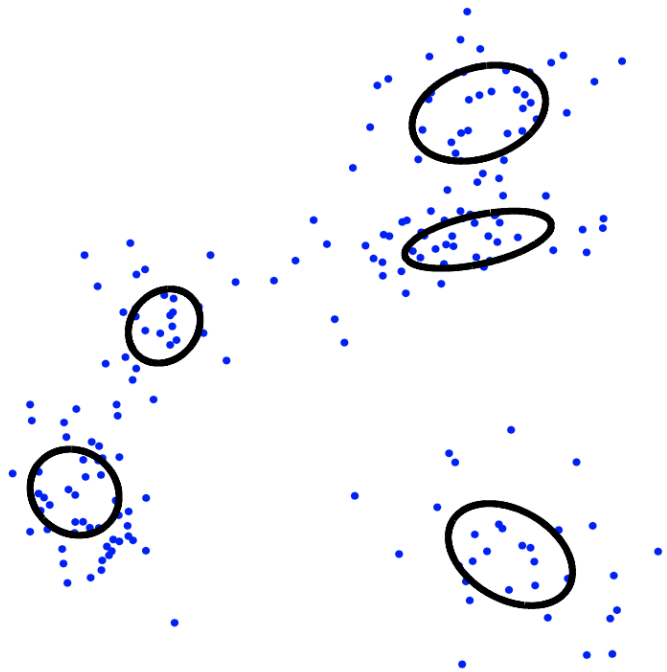
- A generative approach to clustering
  - pick one of K clusters from a distribution $\pi = (\pi_1, \ldots, \pi_K)$
  - generate a data point from a cluster-specific probability distribution
- This yields a finite mixture model:

$$p(x|\phi, \pi) = \sum_{k=1}^{K} \pi_k p(x|\phi_k)$$

  where π and $\phi = (\phi_1, \ldots, \phi_K)$ are the parameters, and here we assume the same parameterized family for each cluster for simplicity.
- Data $\{x_i\}_{i=1}^N$ are assumed to be generated iid from this mixture model.

Example: Gaussian Mixtures

- For Gaussian mixtures, $\phi_k = (\mu_k, \Sigma_K)$ and $p(x|\phi_k)$ is a Gaussian density with mean μ_k and covariance matrix Σ_k



- Mixture models make the assumption that each data point arises from a single mixture component, i.e., the kth cluster is by definition the set of data points arising from the kth mixture component.
- Can capture this explicitly via a latent multinomial variable Z:

$$p(x|\phi,\pi) = \sum_{k=1}^{K} p(Z=k|\pi)p(x|Z=k,\phi)$$
$$= \sum_{k=1}^{K} \pi_k p(x|\phi_k)$$

- Another way to express this: define an underlying measure

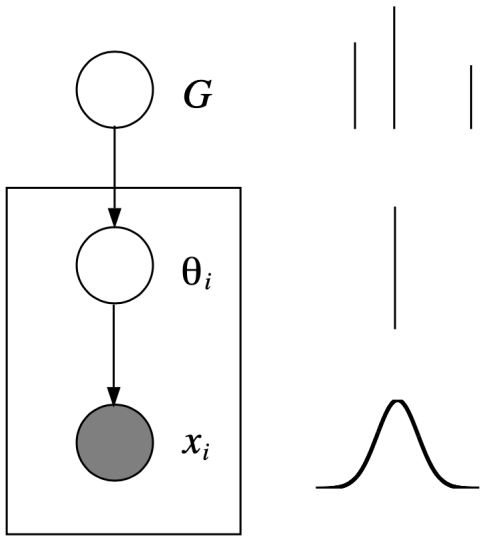
$$G = \sum_{k=1}^{K} \pi_k \delta_{\phi_k}$$

where δ_{ϕ_k} is an *atom* (Dirac delta function) at ϕ_k.

- Now we can redefine the process of obtaining a sampling from a finite mixture model as follows. For $i = 1, \ldots, n$:

$$\theta_i \sim G$$
$$x_i \sim p(\cdot|\theta_i)$$

- Note that each θ_i is equal to one of the underlying ϕ_k. Indeed, the subset of $\{\theta_i\}$ that maps to ϕ_k is exactly the kth cluster



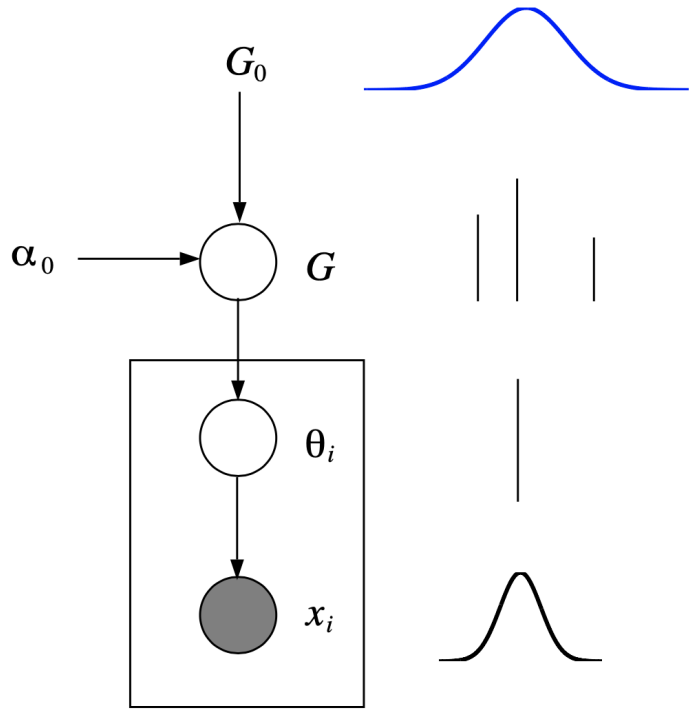
$$
\begin{aligned}
G &= \sum_{k=1}^{K} \pi_k \, \delta_{\phi_k} \\
\theta_i &\sim G \\
x_i &\sim p(\cdot \,|\, \theta_i)
\end{aligned}
$$

Adapted from M. I. Jordan

- Bayesian approaches allow us to integrate out model parameters
- Need to place priors on the parameters ϕ and π
- The choice of prior for ϕ is model-specific; e.g., we may use conjugate normal/inverse-gamma priors for a Gaussian mixture model. Let us denote this prior as G_0.
- What to choose for the mixture weights π? A common choice is a symmetric Dirichlet prior, $\text{Dir}(\alpha_0/K, \ldots, \alpha_0/K)$
  - the symmetry accords with the common assumption of the order-free of the labels of the mixture components
  - the concentration parameter α_0 controls concentration level of the labels

Bayesian Finite Mixture Models

$$
\begin{aligned}
\phi_k &\sim G_0 \\
\pi_k &\sim \mathrm{Dir}(\alpha_0/K, \ldots, \alpha_0/K) \\
G &= \sum_{k=1}^{K} \pi_k \, \delta_{\phi_k} \\
\theta_i &\sim G \\
x_i &\sim p(\cdot \,|\, \theta_i)
\end{aligned}
$$



- Note that G is now a random measure

- Posterior distributions can't be found analytically; nor can predictive distributions (for future observations)
- However, a variety of MCMC sampling algorithms are available
- Use the indicators Z within a Gibbs sampler. Give Z, we know which data points belong to which cluster, so:
  - $p(\pi|Z,\phi)$: standard multinomial-Dirichlet conjugacy
  - $p(\phi|Z,\pi)$: separate updates for each cluster; i.e., for each ϕ_k (and conjugacy of G_0 and $p(\cdot|\phi)$ can make this easy)
  - $p(Z|\pi,\phi)$: multinomial classification
- We can also use variational inference.

- How to choose K, the number of mixture components?
- Various generic model selection methods can be considered: e.g., cross-validation, bootstrap, AIC, BIC, DIC, Laplace, bridge sampling, etc
- Or we can place a parametric prior on K (e.g., Poisson) and use Bayesian methods
- The Dirichlet process provides a nonparametric Bayesian alternative.

- Make sure we always have more clusters than we need.
- How about infinite clusters a priori?

$$p(x|\phi,\pi) = \sum_{k=1}^{\infty} \pi_k p(x|\phi_k)$$

- A finite data set will always use a finite, but random, number of clusters.
- How to choose the prior?
- We need something like a Dirichlet prior, but with an infinte number of components.

Properties of The Dirichlet Distribution

- Relation to gamma distribution: If $\eta_k \sim \text{Gamma}(\alpha_k, \beta)$ independently, then

$$S = \sum_k \eta_k \sim \text{Gamma}\left(\sum_k \alpha_k, \beta\right)$$

and

$$V = (v_1, \ldots, v_k) = (\eta_1/S, \ldots, \eta_k/S) \sim \text{Dir}(\alpha_1, \ldots, \alpha_K)$$

- Therefore, if $(\pi_1, \ldots, \pi_K) \sim \text{Dir}(\alpha_1, \ldots, \alpha_K)$ then

$$(\pi_1 + \pi_2, \pi_3, \ldots, \pi_K) \sim \text{Dir}(\alpha_1 + \alpha_2, \alpha_3, \ldots, \alpha_K)$$

This is known as the collapsing property.

Properties of The Dirichlet Distribution

- The beta distribution is a Dirichlet distribution on the 1-simplex
- Let $(\pi_1, \ldots, \pi_K) \sim \text{Dir}(\alpha_1, \ldots, \alpha_K)$ and $\theta \sim \text{Beta}(\alpha_1 b, \alpha_1(1-b)),\ 0 < b < 1$.
- Then

$$(\pi_1\theta, \pi_1(1-\theta), \pi_2, \ldots, \pi_K) \sim \text{Dir}(\alpha_1 b_1, \alpha_1(1-b_1), \alpha_2, \ldots, \alpha_K)$$

- More generally, if $\theta \sim \text{Dir}(\alpha_1 b_1, \alpha_1 b_2, \ldots, \alpha_1 b_N),\ \sum_i b_i = 1$, then

$$(\pi_1\theta_1, \ldots, \pi_1\theta_N, \pi_2, \ldots, \pi_K) \sim \text{Dir}(\alpha_1 b_1, \ldots, \alpha_1 b_N, \alpha_2, \ldots, \alpha_K)$$

This is known as the splitting property.

Properties of The Dirichlet Distribution

- Renormalization. If $(\pi_1, \ldots, \pi_K) \sim \mathrm{Dir}(\alpha_1, \ldots, \alpha_K)$, and

$$V = (V_2, V_3, \ldots, V_K), \quad V_k = \frac{\pi_k}{\sum_{k \geq 2} \pi_k}$$

- What is the distribution of V?

$$V \sim \mathrm{Dir}(\alpha_2, \ldots, \alpha_K)$$

- All these properties can be easily verified using the aforementioned gamma distribution representation.

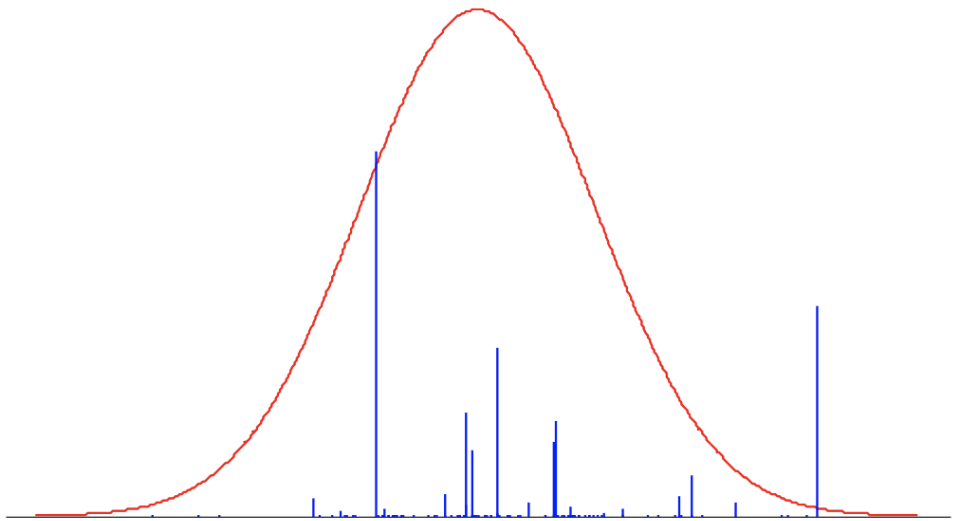
- Let G_0 be a distribution on some space Ω, e.g. a Gaussian distribution on the real line.
- Assume that π, ϕ have the following distributions

$$\phi_k \sim G_0$$
$$\pi \sim \lim_{K \to \infty} \mathrm{Dir}\left(\frac{\alpha_0}{K}, \ldots, \frac{\alpha_0}{K}\right)$$

- Then $G := \sum_{k=1}^{\infty} \pi_k \delta_{\phi_k}$ defines an infinite distribution over G_0.
- We say (informally) that G follows a Dirichlet Process

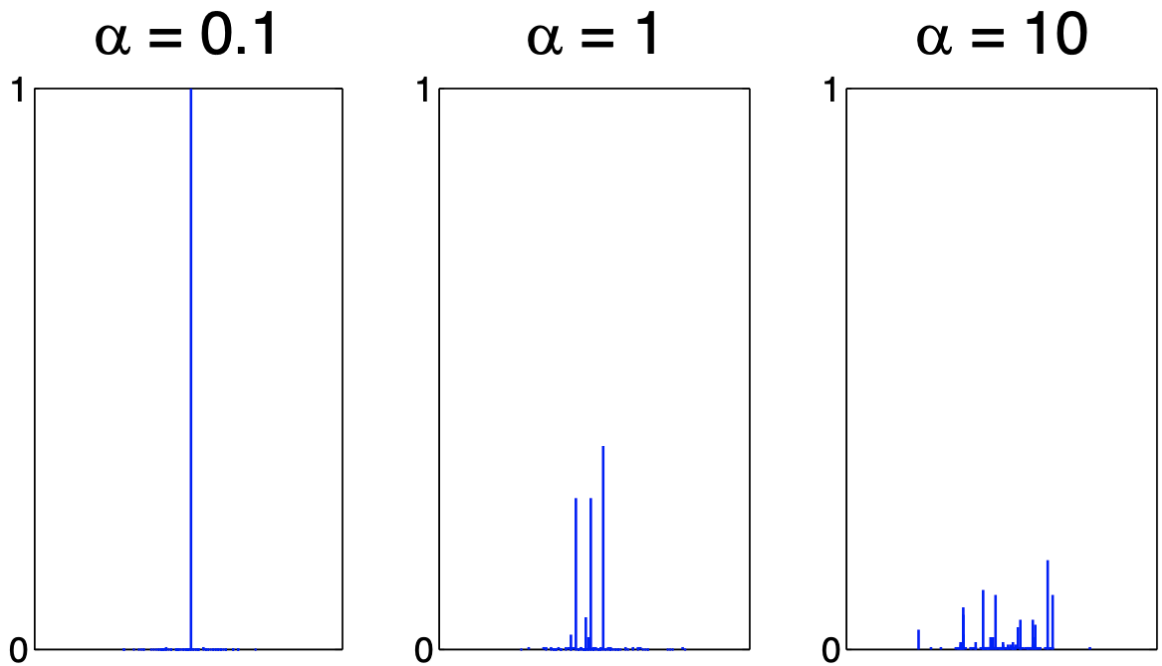
$$G \sim \mathrm{DP}(\alpha_0 G_0)$$

- Samples from the Dirichlet process are *discrete*.
- We call the point masses in the resulting distribution, atoms.



- The *base measure* G_0 determines the *locations* of the atoms.

- The *concentration parameter* α_0 determines the distribution over atom sizes.
- Small values of α_0 gives *sparse* distributions.



Dirichlet Process: A Formal Definition

- Let $(\Omega, \mathcal{B})$ be a measurable space, with G_0 a probability measure on the space, and let α_0 be a positive real number.
- A Dirichlet process is the distribution of a random probability measure G over $(\Omega, \mathcal{B})$ such that, for any finite partition $(A_1, \ldots, A_r)$ of Ω, the random vector $(G(A_1), \ldots, G(A_r))$ follows a finite-dimensional Dirichlet distribution:

$$(G(A_1), \ldots, G(A_r)) \sim \mathrm{Dir}(\alpha_0 G_0(A_1), \ldots, \alpha_0 G(A_r))$$

- We write $G \sim \mathrm{DP}(\alpha_0 G_0)$, and call G_0 the base measure, α_0 the concentration parameter.

- Let $A_1, \ldots, A_K$ be a partition of Ω. Let $G(A_k)$ be the mass assigned by $G \sim \mathrm{DP}(\alpha_0 G_0)$ to partition A_k. Then

$$(G(A_1), \ldots, G(A_K)) \sim \mathrm{Dir}(\alpha_0 G_0(A_1), \ldots, \alpha_0 G_0(A_K))$$

- If we see an observation in the j-th segment, then

$$\begin{aligned}(G(A_1), \ldots, G(A_K) | \theta_1 \in A_j) \\ \sim \mathrm{Dir}(\alpha_0 G_0(A_1), \ldots, \alpha_0 G(A_j) + 1, \ldots, \alpha_0 G_0(A_K)).\end{aligned}$$

- This is true for all possible partitions of Ω.
- Therefore, the posterior distribution of G, given an observation ϕ, is given by

$$G | \theta_1 = \phi \sim \mathrm{DP}(\alpha_0 G_0 + \delta_\phi)$$

Predictive Distribution

- The Dirichlet process clusters observations.
- A new data point can either join an existing cluster, or start a new cluster.
- Question: What is the predictive distribution for a new data point?
- Assume G_0 is a continuous distribution on Ω. This means for every point ϕ in Ω, $G_0(\phi) = 0$.
- First data point:
  - Start a new cluster
  - Sample a parameter $\phi_1 \sim G_0$ for that cluster.

- We have now split our parameter space in two: the singleton ϕ_1, and everything else.
- Let π_1 be the size of atom at ϕ_1.
- The combined mass of all the other atoms is $\pi_* = 1 - \pi_1$.
- According to the DP,

$$(\pi_1, \pi_*) \sim \text{Dir}(0, \alpha_0)$$

- Given $\theta_1 = \phi_1$, the posterior is

$$(\pi_1, \pi_*)|\theta_1 = \phi_1 \sim \text{Dir}(1, \alpha_0)$$

- If we integrate out π_1, we get

$$
\begin{aligned}
p(\theta_2 = \phi_k | \theta_1 = \phi_1) &= \int p(\theta_2 = \phi_k | (\pi_1, \pi_*)) p((\pi_1, \pi_*) | \theta_1 = \phi_1) d\pi_1 \\
&= \int \pi_k \mathrm{Dir}((\pi_1, 1 - \pi_1) | 1, \alpha_0) d\pi_1 \\
&= \mathbb{E}_{\mathrm{Dir}(1, \alpha_0)} \pi_k \\
&= \begin{cases} \frac{1}{1+\alpha_0} & \text{if } k = 1 \\ \frac{\alpha_0}{1+\alpha_0} & \text{for new } k. \end{cases}
\end{aligned}
$$

- Lets say we choose to start a new cluster, and sample a new parameter $\phi_2 \sim G_0$. Let π_2 be the size of the atom at ϕ_2.
- Similarly, the posterior is

$$(\pi_1, \pi_2, \pi_*)|\theta_1 = \phi_1, \theta_2 = \phi_2 \sim \text{Dir}(1, 1, \alpha_0)$$

- If we integrate out $\pi = (\pi_1, \pi_2, \pi_*)$, we get

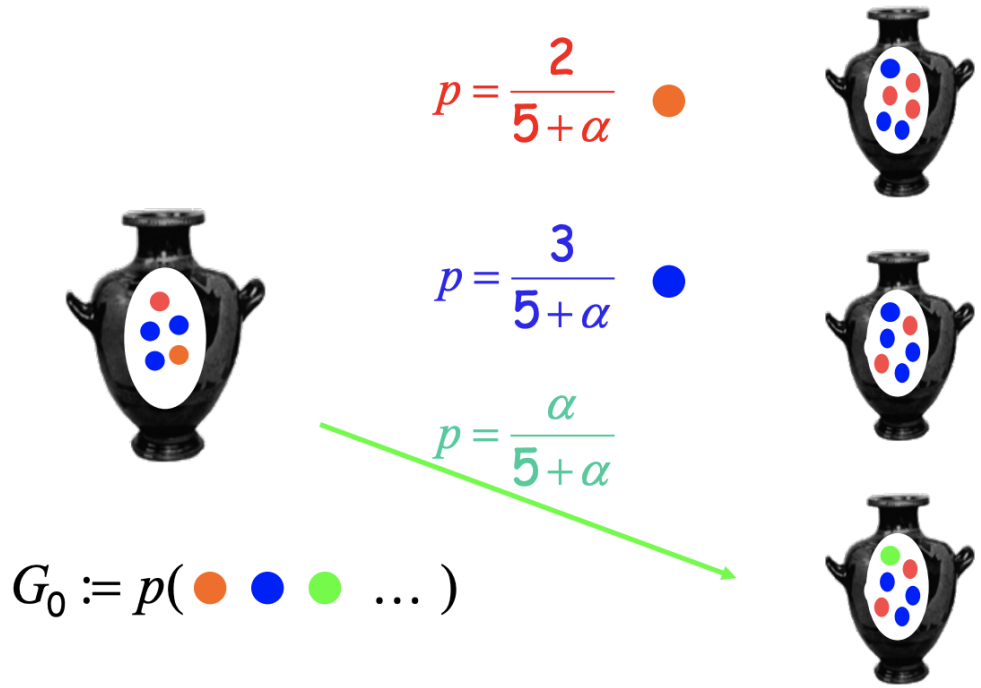
$$\begin{aligned} & p(\theta_3 = \phi_k | \theta_1 = \phi_1, \theta_2 = \phi_2) \\ & \quad = \int p(\theta_3 = \phi_k|\pi) p(\pi|\theta_1 = \phi_1, \theta_2 = \phi_2) d\pi \\ & \quad = \mathbb{E}_{\text{Dir}(1,1,\alpha_0)} \pi_k \\ & \quad = \begin{cases} \frac{1}{2+\alpha_0} & \text{if } k = 1 \\ \frac{1}{2+\alpha_0} & \text{if } k = 2 \\ \frac{\alpha_0}{2+\alpha_0} & \text{for new } k. \end{cases} \end{aligned}$$

Predictive Distribution

- In general, if m_k is the number of times we have seen $X_i = k$, and K is the total number of observed values,

$$
\begin{aligned}
p(\theta_{n+1} = \phi_k | \theta_1, \ldots, \theta_n) &= \int p(\theta_{n+1} = \phi_k | \pi) p(\pi | \theta_1, \ldots, \theta_n) d\pi \\
&= \mathbb{E}_{\mathrm{Dir}(m_1, \ldots, m_K, \alpha_0)} \pi_k \\
&= \begin{cases} \frac{m_k}{n+\alpha_0} & \text{if } k \leq K \\ \frac{\alpha_0}{n+\alpha_0} & \text{for new cluster.} \end{cases}
\end{aligned}
$$

- We tend to see observations that we have seen before, i.e., rich-get-richer property
- We can always add new features, a typical nonparametric behavior.



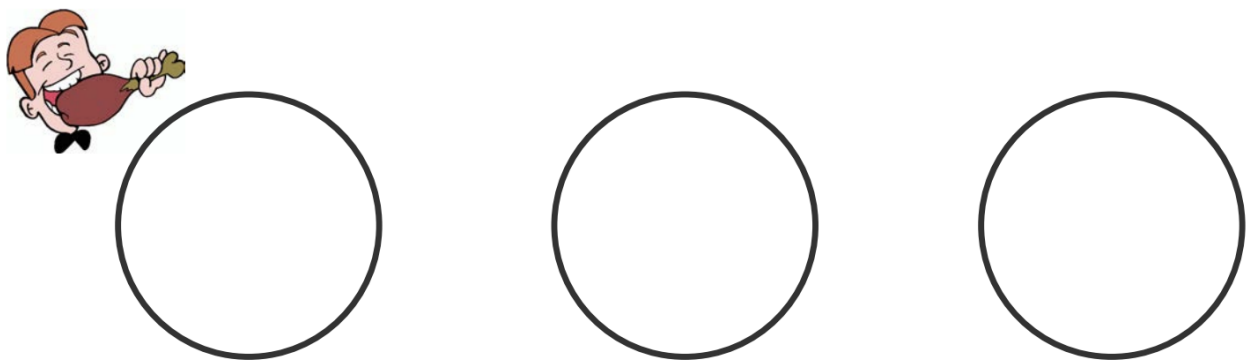
Adapted from Eric Xing

- Joint: $G(\ ) \sim \mathrm{DP}(\alpha_0 G_0)$
- Marginal: $\theta_{n+1}|\theta_{\leq n}, \alpha_0, G_0 \sim \sum_{k=1}^{K} \frac{m_k}{n+\alpha_0}\delta_{\phi_k} + \frac{\alpha_0}{n+\alpha_0}G_0.$

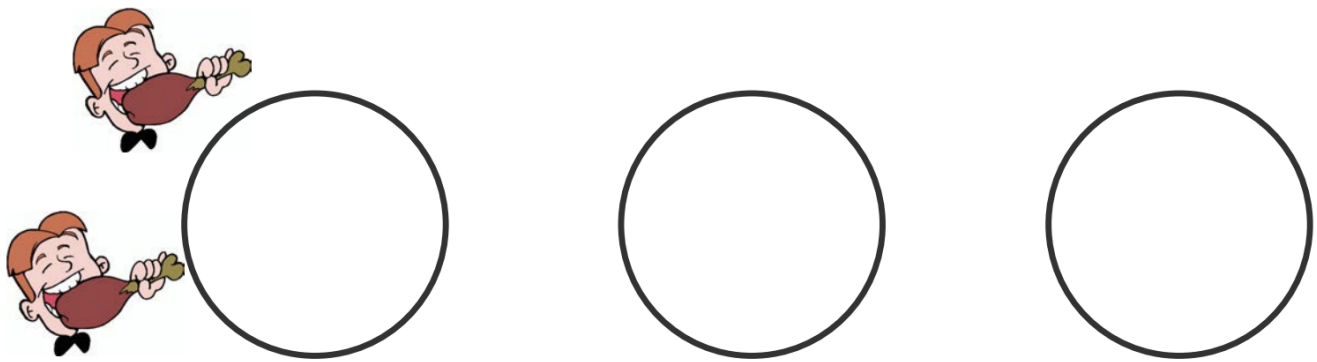
- The resulting distribution over data points can be thought of using the following urn scheme (Blackwell and MacQueen, 1973).
- An urn initially contains a black ball of mass α_0.
- For $n = 1, 2, \ldots$, sample a ball from the urn with probability proportional to its mass.
- If the ball is black, choose a previously unseen color, record that color, and return the black ball plus a unit-mass ball of the new color to the urn.
- If the ball is not black, record it's color and return it, plus another unit-mass ball of the same color, to the urn.

- The distribution over partitions can also be described in terms of the following restaurant metaphor:

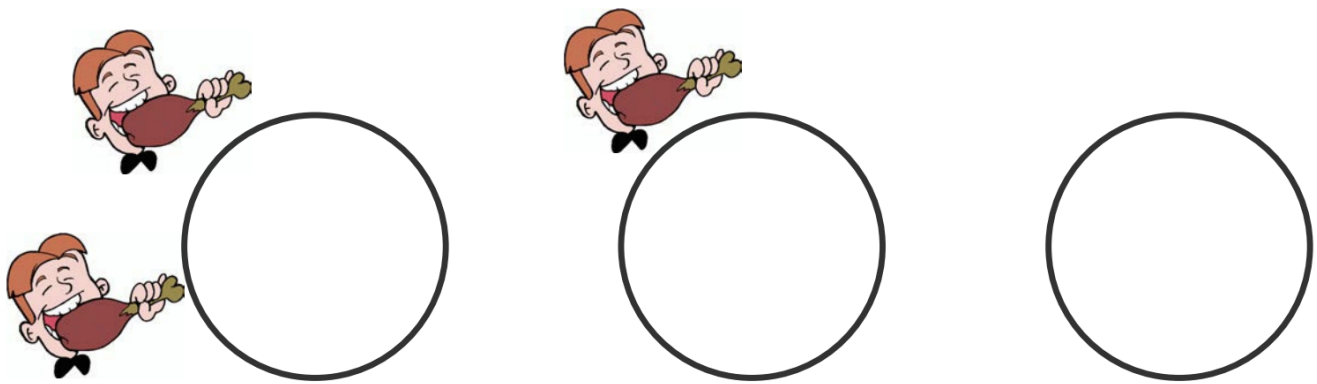
- The distribution over partitions can also be described in terms of the following restaurant metaphor:
- The first customer enters a restaurant, and picks a table.



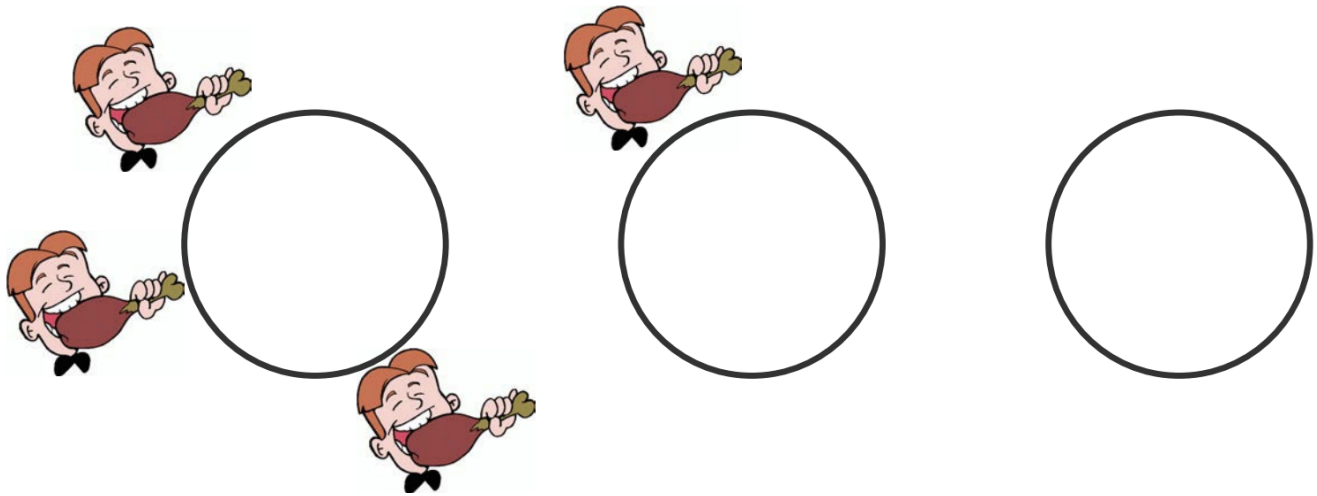
- The distribution over partitions can also be described in terms of the following restaurant metaphor:
- The first customer enters a restaurant, and picks a table.
- The n-th customer enters the restaurant. He sits at an existing table with probability $\frac{m_k}{n-1+\alpha_0}$, where m_k is the number of people sat the table k. He starts a new table with probability $\frac{\alpha_0}{n-1+\alpha_0}$.



- The distribution over partitions can also be described in terms of the following restaurant metaphor:
- The first customer enters a restaurant, and picks a table.
- The n-th customer enters the restaurant. He sits at an existing table with probability $\frac{m_k}{n-1+\alpha_0}$, where m_k is the number of people sat the table k. He starts a new table with probability $\frac{\alpha_0}{n-1+\alpha_0}$.



- The distribution over partitions can also be described in terms of the following restaurant metaphor:
- The first customer enters a restaurant, and picks a table.
- The n-th customer enters the restaurant. He sits at an existing table with probability $\frac{m_k}{n-1+\alpha_0}$, where m_k is the number of people sat the table k. He starts a new table with probability $\frac{\alpha_0}{n-1+\alpha_0}$.



- An interesting fact: the distribution over the clustering of the first N customers does not depend on the order in which they arrived.
- However, the customers are not independent. They tend to sit at popular tables.
- We say that distributions like this are *exchangeable*.

$$p(\theta_1, \ldots, \theta_N) = p(\theta_{\sigma(1)}, \ldots, \theta_{\sigma(n)})$$

- By **de Finetti**'s theorem, there exists a random distribution G and a prior $P(G)$ such that

$$p(\theta_1, \ldots, \theta_N) = \int \prod_{i=1}^{N} G(\theta_i) dP(G)$$

- In our setting, the prior $p(G)$ is just $\mathrm{DP}(\alpha_0 G_0)$, thus establishing existence.

A Second Perspective: Stick Breaking

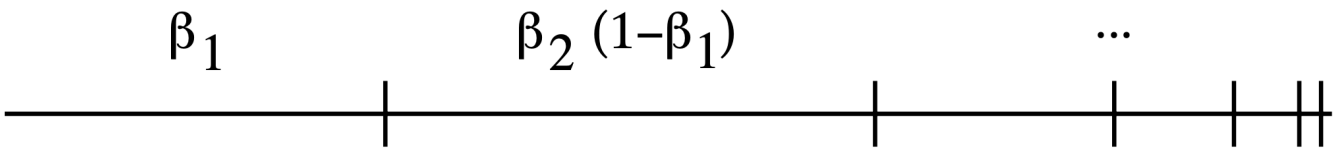
- Define an infinite sequence of Beta random variables:

$$\beta_k \sim \text{Beta}(1, \alpha_0), \quad k = 1, 2, \ldots$$

- Now define an infinite sequence of mixing proportions as:

$$\pi_1 = \beta_1$$
$$\pi_k = \beta_k \prod_{\ell=1}^{k-1} (1 - \beta_\ell), \quad k = 2, 3, \ldots$$

- This can be viewed as breaking off portions of a stick:



- We now have an explicit formula for each π_k:

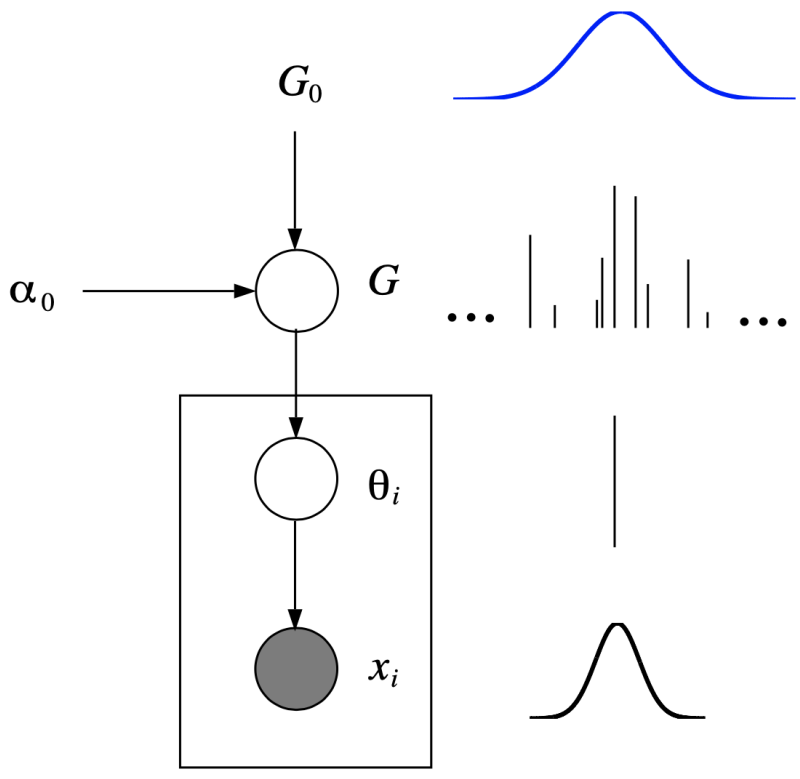
$$\pi_k = \beta_k \prod_{\ell=1}^{k-1} (1 - \beta_\ell)$$

- We can easily see that $\sum_{k=1}^{\infty} \pi_k = 1$:

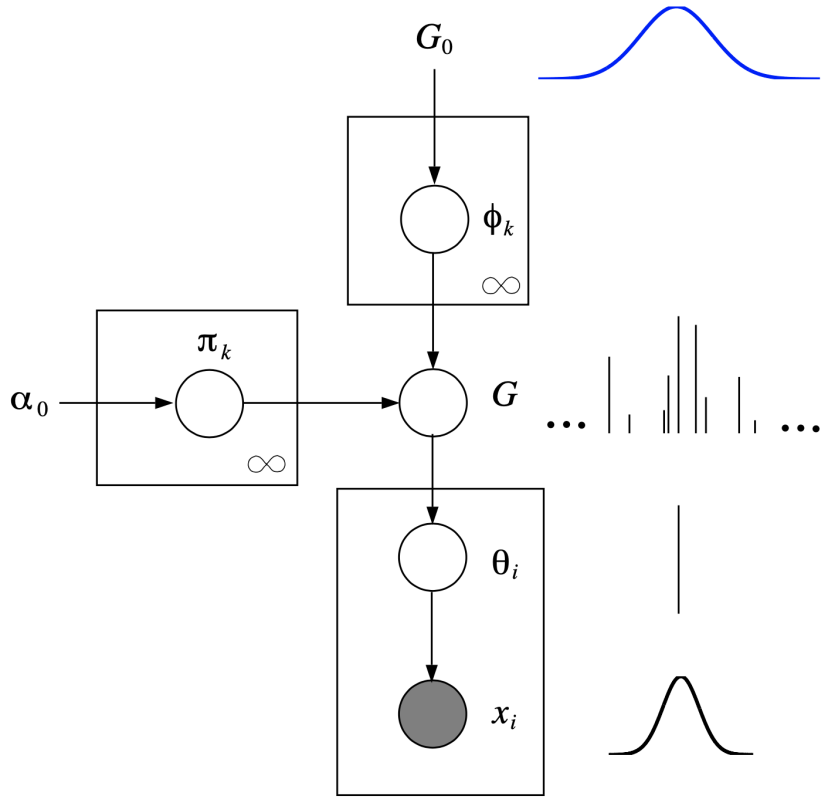
$$\begin{aligned} 1 - \sum_{k=1}^{\infty} \pi_k &= 1 - \beta_1 - \beta_2(1-\beta_1) - \beta_3(1-\beta_1)(1-\beta_2) - \cdots \\ &= (1-\beta_1)(1 - \beta_2 - \beta_3(1-\beta_2) - \cdots) \\ &= \prod_{k=1}^{\infty}(1-\beta_k) = 0 \end{aligned}$$

- Let $\phi_k \sim G_0, \forall k$, $G = \sum_{k=1}^{\infty} \pi_k \delta_{\phi_k}$ has a clean definition as a random measure. In fact,

$$G \sim \mathrm{DP}(\alpha_0 G_0).$$



Polya urn construction



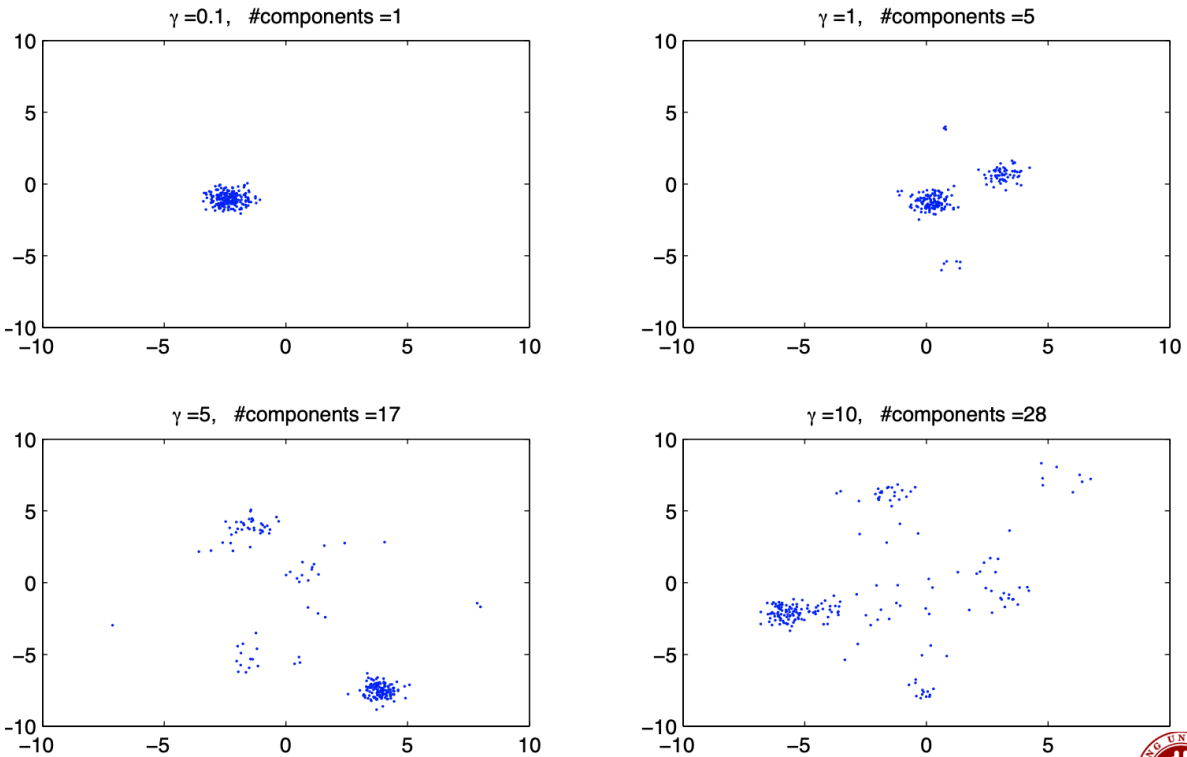
Stick breaking construction

- Now we can use a Dirichlet process as the prior for an unknown mixture distribution (with potentially infinite mixture components).
- Suppose we have $x_1, \ldots, x_n$ observations from some unknown distribution.
- We can model the unknown distribution of x as a mixture of simple distributions of the form $f(\cdot|\theta)$.
- We denote the mixing distribution over θ as G and let the prior over G be a Dirichlet process

$$
\begin{aligned}
x_i|\theta_i &\sim f(\theta_i) \\
\theta_i|G &\sim G \\
G &\sim \mathrm{DP}(\alpha_0 G_0)
\end{aligned}
$$

Samples from DP Mixture Prior

- Multiple subjects can be mapped to the same ϕ. This creates a clustering of subjects.
- The following graphs shows 4 different data sets ($n = 200$) randomly generated from distributions sampled from Dirichlet process mixture priors with α_0.



- We can integrate out G to get the CRP. Note that the CRP is exchangeable, which induces the conditional priors

$$p(\theta_i|\theta_{-i},\alpha_0,G_0)=\frac{\alpha_0}{n-1+\alpha_0}G_0(\theta_i)+\sum_{k=1}^{K^{(-i)}}\frac{m_k^{(-i)}}{n-1+\alpha_0}\delta_{\phi_k^{(-i)}}$$

- Let z_i be the cluster allocation of the i-th data point. The collapsed Gibbs sampler alternates between
  - update z_i

$$p(z_i=k|x_i,z_{-i},\phi_{1:K})\propto\begin{cases} m_k^{(-i)}f(x_i|\phi_k^{(-i)}) & k\le K^{(-i)} \\ \alpha_0\int f(x_i|\theta)dG_0(\theta) & k=K^{(-i)}+1 \end{cases}$$

  - update ϕ_k

$$p(\phi_k|z_{1:n},x_{1:n})\propto G_0(\phi_k)\prod_{i:z_i=k}f(x_i|\phi_k)$$

- If G_0 is conjugate to f, the above steps can be evaluated accurately.

- For the concentration parameter α_0, we have

$$p(K|\alpha_0) \propto \alpha_0^K \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_0 + n)}$$

  where K is the number of unique ϕ's (e.g., the number of clusters).
- Therefore, given K and the prior distribution $P(\alpha_0)$ we can sample from the posterior distribution of α_0 using the MH algorithm or the Gibbs sampling method of Escobar and West (1995).

Problems with The Collapsed Gibbs Sampler

- We are only updating one data point at a time.
- Imagine two "true" clusters are merged into a single cluster, a single data point is unlikely to "break away".
- Getting to the true distribution involves going through low probability states, i.e., mixing can be slow.
- If the likelihood is not conjugate, integrating out parameter values for new features can be difficult.
- Neal (2000) offers a variety of algorithms.

- The stick-breaking representation orders the mixture components so that the weights are stochastically decreasing. For a sufficiently large T, we will have $\sum_{k>T} \pi_k \approx 0$.
- Therefore, we can truncate the stick-breaking construction at a fixed value T and let $\beta_T = 1$.
- This implies $\pi_k = 0, \forall k > T$, and the distribution of

$$G_T = \sum_{k=1}^{T} \pi_k \delta_{\phi_k}$$

is known as a truncated Dirichlet process.

- Variational distance between distributions of marginals from a DP and from its truncation at T is approximately $4n \exp(-(T-1)/\alpha_0)$. T doesn't have to be very large to get a good approximation.

Blocked Gibbs Sampler

- State of the Markov chain: $(\beta_{1:T-1}, \phi_{1:T}, z_{1:n})$.
- Update z_i by multinomial sampling with

$$p(z_i = k|\beta, \phi, x_i) \propto \pi_k f(x_i|\phi_k)$$

- Update β_k by sampling from the conditional posterior

$$\beta_k \sim \text{Beta}(1 + m_k, \alpha_0 + \sum\nolimits_{j>k} m_j)$$

- Update ϕ_k by sampling from the conditional posterior

$$p(\phi_k|z_{1:n}, x_{1:n}) \propto G_0(\phi_k) \prod_{i:z_i=k} f(x_i|\phi_k)$$

- One can monitor $\max_i z_i$ to verify that truncation at T is good enough, and increase T if necessary.

- We can also use truncated steak-breaking representation to form a mean field approximation of DP mixtures

$$q(\beta, \phi, z) = \prod_{i=1}^{n} q(z_i|w_i) \prod_{k=1}^{T} q(\phi_k|\tau_k) \prod_{k=1}^{T-1} q(\beta_k|\gamma_k)$$

- For a conjugate DP mixture in the exponential family

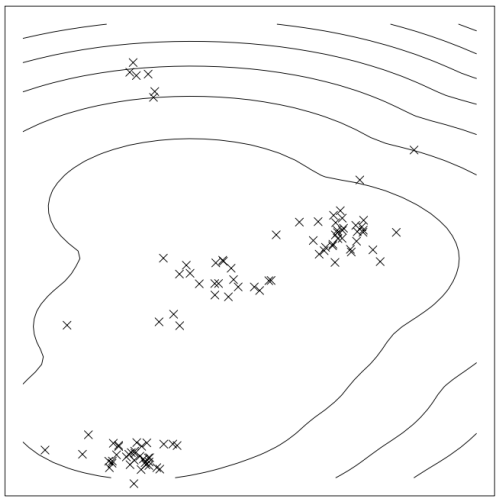
$$\gamma_{k,1} = 1 + \sum_{i=1}^{n} w_{i,k}, \quad \gamma_{k,2} = \alpha_0 + \sum_{i=1}^{n} \sum_{j>k} w_{i,j}$$
$$\tau_{k,1} = \lambda_1 + \sum_{i=1}^{n} w_{i,k} t(x_i), \quad \tau_{k,2} = \lambda_2 + \sum_{i=1}^{n} w_{i,k}$$
$$w_{i,k} \propto \exp(S_k)$$

where

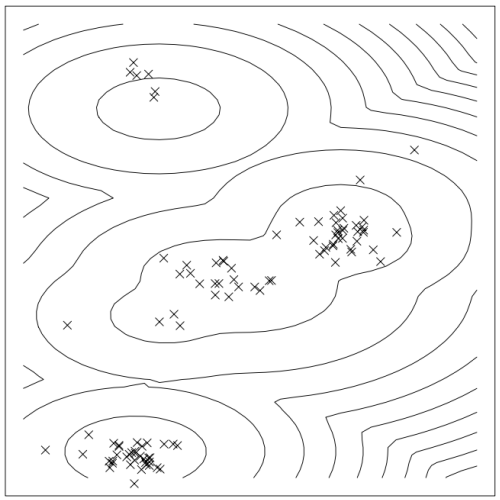
$$S_k = \mathbb{E} \log \beta_k + \sum_{j<k} \mathbb{E} \log(1 - \beta_j) + \mathbb{E} \phi_k^T t(x_i) - \mathbb{E} A(\phi_k)$$

Example: DP Gaussian Mixture

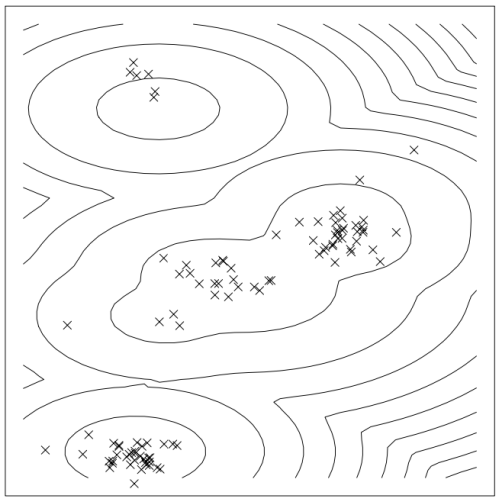
- The approximate predictive distribution given by variational inference at different stages of the algorithm. The data are 100 points generated by a Gaussian DP mixture model with fixed diagonal covariance.



Initial state



1st iteration



5th (and last) iteration

References

- Antoniak, C. (1974). Mixtures of Dirichlet processes with applications to Bayesian nonparametric problems. The Annals of Statistics, 2(6):1152–1174..
- Blackwell, D. and MacQueen, J. (1973). Ferguson distributions via Pólya urn schemes. The Annals of Statistics, 1(2):353–355.
- Ferguson, T. (1973). A Bayesian analysis of some nonparametric problems. The Annals of Statistics, 1:209–230.
- Escobar, M. and West, M. (1995). Bayesian density estimation and inference using mixtures. Journal of the American Statistical Association, 90:577–588.

References

- Neal, R. (2000). Markov chain sampling methods for Dirichlet process mixture models. Journal of Computational and Graphical Statistics, 9(2):249–265.
- Blei, D. M. and Jordan, M. I. (2005). Variational inference for Dirichlet process mixtures. Bayesian Analysis, 1(1):121-144.
- Y. W. Teh, M. I. Jordan, M. J. Beal, and D. M. Blei. Hierarchical Dirichlet processes. Journal of the American Statistical Association, 101(476):1566–1581, 2006.