Methods

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Methods

We have N observations X_1, \ldots, X_N , and for each X_i , we have following assumption with fixed σ^2 .

$$X_i \sim \mathcal{N}(\mu_i, \sigma^2)$$

We consider X_i and X_j should be in one cluster, if $\mu_i = \mu_j$. We want to propose a prior \mathcal{H} for μ . If \mathcal{H} is a continuous distribution, we have $Pr(\mu_i = \mu_j) = 0$, which is infeasible for clustering. Therefore, we introduce a discrete approximation for our prior by using Dirichlet Process(DP).

Dirichlet Process (DP)

We have a measure space (Θ, Σ) . Define a measurable finite partitioning of Θ to be a finite collection of sets A_1, A_2, \ldots, A_K such that:

(1) Finite: $K < \infty$. (2) Measureable: $A_k \in \Sigma$. (3) Disjoint: $A_j \cap A_k = \emptyset, \forall j \neq k$. (4) Complete: $\bigcup_k A_k = \Theta$.

A Dirichlet process is a random probability measure G over a (Θ, Σ) with property that given any measurable finite partitioning of Θ , we have

$$[G(A_1), \ldots, G(A_K)] \sim Dirichlet(\alpha H(A_1), \ldots, \alpha H(A_K))$$

where α is scale, and H is base measure, and $G \sim DP(\alpha, H)$ will be discrete. [1]

Dirichlet Process Gaussian Mixture Model (DPGMM)

With introduction of DP, we can reformulate our model as following with given σ^2 , α , μ_0 , σ_0^2 .

$$X_i \sim \mathcal{N}(\mu_i, \sigma^2)$$

$$\mu_i | G \sim G$$

$$G \sim DP(\alpha, \mathcal{N}(\mu_0, \sigma_0^2))$$

Notation

We slice space of μ into K partitions, and use Z_i to indicate which partition μ_i falls in, which is our cluster assignment for X_i .

$$\begin{split} Z_i &= k \Leftrightarrow \mu_i \text{ in kth partition} \quad \text{where } k \in [1, 2, \dots, K] \\ p_k &\triangleq P(Z_j = k) \quad \forall j \in [1, 2, \dots, N] \\ p &\triangleq \{p_1, \dots, p_K\}, \quad -i \triangleq \{1, 2, \dots, i - 1, i + 1, \dots, N\} \\ n_{k, -i} &= \text{count of } j \quad \text{s.t. } Z_j = k \text{ and } j \neq i \end{split}$$

If we have infinite partitions $K \to \infty$, we can rewrite our DPGMM model as following:

$$X_{i}|\mu \sim \mathcal{N}(\mu_{i}, \sigma^{2})$$

$$Z_{i}|p \sim Discrete(p_{1}, \dots, p_{K})$$

$$\mu_{i} \sim \mathcal{N}(\mu_{0}, \sigma_{0}^{2})$$

$$p \sim Dir(\alpha/K, \dots, \alpha/K)$$

Predictive Distribution

We have following predictive distribution for Z_i , and detail of result derivation is discussed in appendix A.

$$P(Z_{i} = m | Z_{-i}) = \frac{P(Z_{i} = m, Z_{-i})}{P(Z_{-i})}$$

$$= \frac{\int_{p} P(Z_{i} = m, Z_{-i} | p_{1}, \dots, p_{K}) P(p_{1}, \dots, p_{K}) dp}{\int_{p} P(Z_{-i} | p_{1}, \dots, p_{K}) P(p_{1}, \dots, p_{K}) dp}$$

$$= \frac{\frac{\alpha}{K} + n_{m,-i}}{\alpha + N - 1}$$
[A.1]

Chinese Restaurant Process (CRP)

Based on pervious predictive distribution, when $K \to \infty$, we have Chinese restaurant process.

$$P(Z_i = m | Z_{-i}) = \frac{n_{m,-i}}{\alpha + N - 1} \quad existing \ cluster \ m$$

$$P(Z_i = new | Z_{-i}) = \frac{\alpha}{\alpha + N - 1} \quad new \ cluster$$

Gibbs Sampler for DPGMM

Based on exchangeability, we have following predictive probability for Gibbis sampling [2] [3] [4]. Detail of derivation for new cluster case is discussed in appendix A.

$$P(Z_{i} = m | Z_{-i}, X) \propto P(Z_{i} = m | Z_{-i}, \alpha) \cdot P(X_{i} | Z_{i} = m, \mu_{i})$$

$$\propto \begin{cases} n_{m,-i} \cdot \mathcal{N}(x_{i}; \mu_{[m]}, \sigma^{2}) & existing cluster m \\ \alpha \int_{\mu} Pr(X_{i} | \mu) \cdot Pr(\mu | \mu_{0}) = \alpha \mathcal{N}(x_{i}; \mu_{0}, \sigma^{2} + \sigma_{0}^{2}) & new cluster \end{cases}$$

$$where \quad \mu_{[m]} = \mu \text{ of cluster } m$$

$$[A.2]$$

Sampling Algorithm

Initialization

Assign all data in one cluster s.t. $Z_1^{(0)} = Z_2^{(0)} = \cdots = Z_n^{(0)} = 1$, and $K^{(0)} = 1$. Sample $\mu_{[1]}^{(0)}$ based on posterior of $\mu|X,Z$ (A.3), where n_l is count for all $Z_l = j$, detail discussed in appendix A.

Run detail

For i in $[1, \dots, N]$ sample $Z_i^{(t+1)}$ based on

$$P(Z_i^{(t+1)} = m) \propto \begin{cases} n_{m,-i}^{(t)} \cdot \mathcal{N}(x_i; \mu_{[m]}^{(t)}, \sigma^2) & existing cluster \ m \\ \alpha \mathcal{N}(x_i; \mu_0, \sigma^2 + \sigma_0^2) & new \ cluster \quad s.t. \quad m = K+1 \end{cases}$$

K = K + 1 each time if our sampled assignment is new. After sampling assignment, we sample $\mu_{[k]}^{(t+1)}$ for all $k \in [1, ..., K]$ based on

$$P(\mu_{[k]}^{(t+1)}|X_l, where Z_l^{(t+1)} = k) \sim \mathcal{N}(\frac{\sum_{\sigma^2}^{x_l} + \frac{\mu_0}{\sigma_0^2}}{\frac{n_k^{(t+1)}}{\sigma^2} + \frac{1}{\sigma_0^2}}, [\frac{n_k^{(t+1)}}{\sigma^2} + \frac{1}{\sigma_0^2}]^{-1})$$
[A.3]

Appendix A

A.1

$$\begin{split} P(Z_i = m | Z_{-i}) &= \frac{P(Z_i = m, Z_{-i})}{P(Z_{-i})} \\ &= \frac{\int_p P(Z_i = m, Z_{-i} | p_1, \dots, p_K) P(p_1, \dots, p_K) dp}{\int_p P(Z_{-i} | p_1, \dots, p_K) P(p_1, \dots, p_K) dp} \\ P(Z_i = m, Z_{-i} | p_1, \dots, p_K) &= p_m^{n_m, -i+1} \prod_{k=1}^K p_k^{n_k, -i} \end{split}$$

Numerator

Therefore, we can write our numerator of the predictive distribution into the following form,

$$\begin{split} numerator &= \int_{p} P(Z_{i} = m, Z_{-i} | p_{1}, \dots, p_{K}) P(p_{1}, \dots, p_{K}) dp \\ &= \int_{p} [p_{m}^{n_{m,-i}+1} \prod_{k=1, k \neq m}^{K} p_{k}^{n_{k,-i}}] \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K})} \prod_{k=1}^{K} p_{k}^{\frac{\alpha}{K}-1} dp \\ &= \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K})} \int_{p} [p_{m}^{\frac{\alpha}{K}+n_{m,-i}+1-1} \prod_{k=1, k \neq m}^{K} p_{k}^{\frac{\alpha}{K}+n_{k,-i}-1}] dp \\ &= \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K})} \frac{\Gamma(\frac{\alpha}{K}+n_{m,-i}+1-1) \cdot \prod_{k=1}^{K} \Gamma(\frac{\alpha}{K}+n_{k,-i})}{\Gamma(\frac{\alpha}{K}+n_{m,-i}+1+\sum_{k=1, k \neq m}^{K} (\frac{\alpha}{K}+n_{k,-i}))} \cdot \end{split}$$

where $[p_m^{\frac{\alpha}{K}+n_{m,-i}+1-1}\prod_{k=1,k\neq m}^K p_k^{\frac{\alpha}{K}+n_{k,-i}-1}]$ is the kernel of $Dir(\frac{\alpha}{K}+n_{1,-i},\ldots,\frac{\alpha}{K}+n_{m,-i}+1,\ldots,\frac{\alpha}{K}+n_{K,-i})$.

Denominator

$$\begin{aligned} denominator &= \int_{p} P(Z_{-i}|p_{1},\ldots,p_{K})P(p_{1},\ldots,p_{K})dp \\ &= \int_{p} [\prod_{k=1}^{K} p_{k}^{n_{k,-i}}] \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K})} \prod_{k=1}^{K} p_{k}^{\frac{\alpha}{K}-1} dp \\ &= \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K})} \int_{p} \prod_{k=1}^{K} p_{k}^{\frac{\alpha}{K}+n_{k,-i}-1} dp \\ &= \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K})} \frac{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K}+n_{k,-i})}{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K}+n_{k,-i})} \int_{p} \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K}+n_{k,-i})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K}+n_{k,-i})} \prod_{k=1}^{K} p_{k}^{\frac{\alpha}{K}+n_{k,-i}-1} dp \end{aligned}$$

We recognize Dirichlet kernel $Dir(\frac{\alpha}{K} + n_{1,-i}, \dots, \frac{\alpha}{K} + n_{K,-i})$

$$denominator = \frac{\Gamma(\sum_{k=1}^{K} \frac{\alpha}{K})}{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K})} \frac{\prod_{k=1}^{K} \Gamma(\frac{\alpha}{K} + n_{k,-i})}{\Gamma(\sum_{k=1}^{K} (\frac{\alpha}{K} + n_{k,-i}))}$$

Predictive Distribution

$$\begin{split} P(Z_i = m | Z_{-i}) &= \frac{numerator}{denominator} \\ &= \frac{\frac{\Gamma(\sum_{k=1}^K \frac{\alpha}{K})}{\prod_{k=1}^K \Gamma(\frac{\alpha}{K} + n_{m,-i} + 1) \cdot \prod_{k=1}^K \Gamma(\frac{\alpha}{K} + n_{k,-i})}{\prod_{k=1}^K \Gamma(\frac{\alpha}{K} + n_{m,-i} + 1 + \sum_{k=1, k \neq m}^K (\frac{\alpha}{K} + n_{k,-i}))}}{\frac{\Gamma(\sum_{k=1}^K \frac{\alpha}{K})}{\prod_{k=1}^K \Gamma(\frac{\alpha}{K} + n_{k,-i})} \frac{\Gamma(\sum_{k=1}^K \frac{\alpha}{K} + n_{k,-i})}{\prod_{k=1}^K \Gamma(\frac{\alpha}{K} + n_{k,-i})}} \\ &= \frac{\Gamma(\frac{\alpha}{K} + n_{m,-i} + 1) \cdot \prod_{k=1}^K \Gamma(\frac{\alpha}{K} + n_{k,-i}) \cdot \Gamma(\sum_{k=1}^K (\frac{\alpha}{K} + n_{k,-i}))}{\prod_{k=1}^K \Gamma(\frac{\alpha}{K} + n_{k,-i}) \cdot \Gamma(\sum_{k=1}^K (\frac{\alpha}{K} + n_{k,-i}))} \\ &= \frac{\Gamma(\frac{\alpha}{K} + n_{m,-i} + 1) \cdot \Gamma(\sum_{k=1}^K (\frac{\alpha}{K} + n_{k,-i}))}{\Gamma(\frac{\alpha}{K} + n_{m,-i}) \Gamma(1 + \sum_{k=1}^K (\frac{\alpha}{K} + n_{k,-i}))} \\ &= \frac{\frac{\alpha}{K} + n_{m,-i}}{\sum_{k=1}^K (\frac{\alpha}{K} + n_{k,-i})} = \frac{\frac{\alpha}{K} + n_{m,-i}}{\sum_{k=1}^K \sum_{k=1}^K n_{k,-i}} \\ &= \frac{\frac{\alpha}{K} + n_{m,-i}}{\alpha + n_{-1}} \\ &= \frac{\frac{\alpha}{K} + n_{m,-i}}{\alpha + n_{-1}} \end{split}$$

A.2

Given $X_i \sim \mathcal{N}(\mu_i, \sigma^2)$, and $\mu_i \sim \mathcal{N}(\mu_0, \sigma_0^2)$

$$\begin{split} P(X_i|Z_i = new, \mu_i) &= \int_{\mu_i} Pr(X_i|\mu_i) \cdot Pr(\mu_i|\mu_0) d\mu_i \\ &\propto \int_{\mu_i} exp[-\frac{1}{2\sigma^2}(x_i - \mu_i)^2] exp[-\frac{1}{2\sigma_0^2}(\mu_i - \mu_0)^2] d\mu_i \\ &= \int_{\mu_i} exp[-\frac{1}{2}(\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2})(\mu_i - \frac{\frac{\mu_0}{\sigma_0^2} + \frac{x_i}{\sigma^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2}})^2] d\mu_i \cdot exp[-\frac{1}{2}(\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2})(\frac{\frac{\mu_0^2}{\sigma_0^2} + \frac{x_i^2}{\sigma^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2}})^2] \end{split}$$

We recognize normal kernel $\mathcal{N}(\frac{\frac{\mu_0}{\sigma_0^2} + \frac{x_i}{\sigma^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2}}, (\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2})^{-1})$

$$\begin{split} P(X_i|Z_i = new, \mu_i) &\propto exp[-\frac{1}{2}(\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2})(\frac{\frac{\mu_0^2}{\sigma_0^2} + \frac{x_i^2}{\sigma^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2}} - \{\frac{\frac{\mu_0}{\sigma_0^2} + \frac{x_i}{\sigma^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2}}\}^2] \\ &= exp[-\frac{1}{2}(\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2})^{-1}((\frac{\mu_0^2}{\sigma_0^2} + \frac{x_i^2}{\sigma^2})(\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2}) - (\frac{\mu_0}{\sigma_0^2} + \frac{x_i}{\sigma^2})^2)] \\ &\propto exp[-\frac{1}{2}(\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2})^{-1}(\frac{x_i^2}{\sigma^2\sigma_0^2} - 2\frac{x_i\mu_0}{\sigma^2\sigma_0^2})] \\ &= exp[-\frac{1}{2}(\frac{\sigma^2\sigma_0^2}{\sigma_0^2} + \frac{\sigma^2\sigma_0^2}{\sigma^2})^{-1}(x_i^2 - 2x_i\mu_0)] \\ &\propto exp[-\frac{1}{2}\frac{1}{\sigma_0^2 + \sigma^2}(x_i - \mu_0)^2] \\ &\sim \mathcal{N}(\mu_0, \sigma^2 + \sigma_0^2) \end{split}$$

A.3

Likelihood

$$L(X_l|\mu_{[k]}) \propto \prod exp(\frac{1}{2\sigma^2}(x_l - \mu_{[k]})^2) = exp(\frac{1}{2\sigma^2}\sum (x_l - \mu_{[k]})^2)$$

Prior

$$\pi(\mu_{[k]}|\mu_0, \sigma_0^2) \propto exp(\frac{1}{2\sigma_0^2}(\mu_{[k]} - \mu_0)^2)$$

Posterior

$$P(\mu_{[k]}|X_{l}, where Z_{l} = k) \propto L(X_{l}|\mu_{[k]})\pi(\mu_{[k]}|\mu_{0}, \sigma_{0}^{2})$$

$$= exp(\frac{1}{2\sigma^{2}}\sum(x_{l} - \mu_{[k]})^{2})exp(\frac{1}{2\sigma_{0}^{2}}(\mu_{[k]} - \mu_{0})^{2})$$

$$\propto exp[-\frac{1}{2}(\frac{1}{\sigma_{0}^{2}} + \frac{n_{k}}{\sigma^{2}})(\mu_{[k]} - \frac{\frac{\mu_{0}}{\sigma_{0}^{2}} + \sum_{\sigma^{2}} x_{l}}{\frac{1}{\sigma_{0}^{2}} + \frac{n_{k}}{\sigma^{2}}})^{2}]$$

$$\sim \mathcal{N}(\frac{\frac{\mu_{0}}{\sigma_{0}^{2}} + \sum_{\sigma^{2}} x_{l}}{\frac{1}{\sigma_{0}^{2}} + \frac{n_{k}}{\sigma^{2}}}, (\frac{1}{\sigma_{0}^{2}} + \frac{n_{k}}{\sigma^{2}})^{-1})$$

Reference

- [1] Ferguson. (1973). "A Bayesian Analysis of Some Nonparametric Problems" Annals of Statistics
- [2] David M. Blei, Michael I. Jordan. (2006). "Variational Inference for Dirichlet Process Mixtures" Bayesian Analysis
- [3] Radford M. Neal. (2000). "Markov Chain Sampling Methods for Dirichlet Process Mixture Models" Journal of Computational and Graphical Statistics

[4] Samuel Harris. (2015) " Dirichlet Process Gaussian Mixture Model Gibbs Sampler for a 1-dimensional Behavioural Time Series Segmentation"