

Clustering - How to choose K?

- Ad hoc approaches: data-driven, but little theory

- Methods based on maximizing objective functions (M-estimators)

e.g. clustering via K-means, spectral clustering has frequentist guarantees but hard to be data-driven

- Parametric methods such as AIC, BIC requires hidden assumptions

Model-based approach:

$$P(X|\phi) = \sum_{k=1}^K \pi_k P(X|\phi_k)$$

Let $G = \sum_{k=1}^K \pi_k \delta_{\phi_k}$ mixing measure.

Model: $\phi | G \sim G$
 $X | \phi \sim P(X|\phi)$

G Random. Need a prior dist on G.

want K unbounded ($K = \infty$) \Rightarrow Stick-breaking prior.

This is a dist over G of form:

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

$\left\{ \begin{array}{l} \pi \text{ Random} \\ \phi \text{ Random} \\ \sum \pi_k = 1 \end{array} \right.$

Chinese Restaurant Process (CRP)

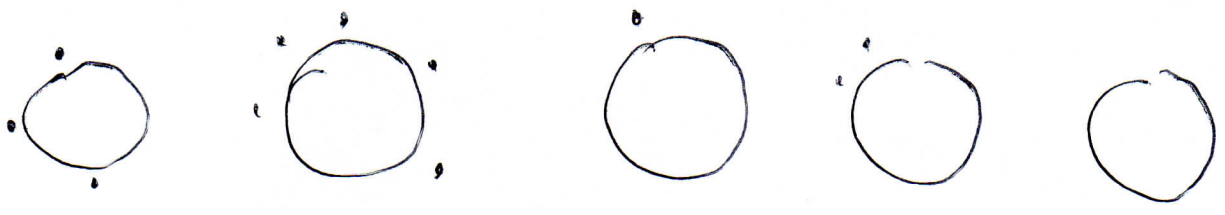
A Random process in which customers sit down in a Chinese Restaurant with infinite number of tables.

CRP: - first customer sits at the first table
 - m-th subsequent customer sits at a table drawn from the following dist:

$$P(\text{sits at previously occupied table } i) \propto n_i$$

$$P(\text{sits in a new (unoccupied) table}) \propto \alpha_0$$

n_i : # customers sitting at table i (among previous $m-1$ customers)



CRP and Clustering

CRP induces a partition of customers into disjoint clusters (subsets)
 dist on and # of clusters (tables)

Let π_k be the proportion of customers sitting at table k .
 $\phi_k \sim G_0$ (because π_k 's, ϕ_k 's are).

Then we obtained a Random measure. $G = \sum_{k=1}^{\infty} \pi_k \delta_{\phi_k}$
 What can we say about G ?

Polya urn model CRP is a particular example of a general class of prob. models known as Polya urn.

~~Let $\theta_1, \dots, \theta_n \sim G$ iid G . there are duplicates among the θ_i 's~~ \Rightarrow The Polya urn model is as follows:

$$\theta_1 \sim G_0$$

$$\theta_i | \theta_1, \dots, \theta_{i-1} \sim \alpha_0 G_0 + \sum_{j=1}^{i-1} \delta_{\theta_j}$$

$$P(\theta_1, \theta_2) = P(\theta_1) P(\theta_2 | \theta_1)$$

$$\propto P(\theta_1) (\alpha_0 G_0(d\theta_2) + \sum_{j=1}^2 \delta_{\theta_1}(\theta_2))$$

$$\propto \alpha_0 G_0(d\theta_1) G_0(d\theta_2) + G_0(d\theta_1) \mathbb{1}(\theta_1 = \theta_2).$$

$$\Rightarrow P(\theta_1, \theta_2) = P(\theta_2, \theta_1).$$

$$P(\theta_1, \theta_2, \theta_3) = P(\theta_1, \theta_2) P(\theta_3 | \theta_1, \theta_2)$$

$$= P(\theta_2, \theta_1) P(\theta_3 | \theta_2, \theta_1) = P(\theta_2, \theta_1, \theta_3)$$

in general $\theta_1, \theta_2, \dots, \theta_n, \dots$ are infinitely exchangeable!

By De Finetti's thm \Rightarrow a random mixing dist G s.t

$$\theta_1, \dots, \theta_n | G \stackrel{iid}{\sim} G.$$

So that $P(\theta_1, \dots, \theta_n) = \int \prod_{i=1}^n P(\theta_i | G) d\pi(G)$

What is G ?

Stick-breaking process:



Let $\beta_k \stackrel{iid}{\sim} \text{Beta}(1, \alpha_0)$ $k=1, 2, \dots$

Define $\pi_1 = \beta_1$

$$\pi_k = \beta_k \prod_{l=1}^{k-1} (1 - \beta_l) \quad k=2, 3, \dots$$

Easy to check that $\sum_{k=1}^{\infty} \pi_k = 1$. (Breaking a stick to small pieces using beta proportions)

$$1 - \sum_{k=1}^K \pi_k = 1 - \beta_1 - \beta_2(1 - \beta_1) - \beta_3(1 - \beta_1)(1 - \beta_2)$$

$$= (1 - \beta_1)(1 - \beta_2) - \beta_3(1 - \beta_1)(1 - \beta_2)$$

$$\dots$$

$$= (1 - \beta_1) \dots (1 - \beta_K) \rightarrow 0 \text{ as } K \rightarrow \infty$$

Thm: Let $G = \sum_{k=1}^{\infty} \pi_k \delta_{\phi_k}$ where $\phi_k \stackrel{iid}{\sim} G_0$ then this is the ~~form~~ ^{dist} G that describes Polya's urn

In fact the random measure G is called a **Pitriehler Process** (4)
 where does Dirichlet come in? Hint: Beta dist was used

Recall Dirichlet Dist (finite) & conjugacy (Dir. Multinomial),

$$P(\pi | \alpha) = \frac{\Gamma(\sum \alpha_i)}{\prod \Gamma(\alpha_i)} \pi_1^{\alpha_1} \dots \pi_k^{\alpha_k} \quad (k < \infty)$$

$$\pi | \alpha \sim \text{Dir}(\alpha)$$

Let $\psi_1, \dots, \psi_n | \pi \stackrel{iid}{\sim} \text{Mult}(\pi) \quad \psi_i \in \{1, \dots, k\}$

$$\begin{aligned} \text{Then } P(\psi_1, \dots, \psi_n) &= \int \prod_{i=1}^n P(\psi_i | \pi) dP(\pi | \alpha) \\ &\propto \int \prod_{k=1}^K \pi_k^{n_k} \prod_{k=1}^K \pi_k^{\alpha_k} d\pi \propto \int \prod_{k=1}^K \pi_k^{n_k + \alpha_k} d\pi \\ &= \frac{\Gamma(\alpha_1 + \dots + \alpha_k)}{\Gamma(\alpha_1) \dots \Gamma(\alpha_k)} \frac{\Gamma(\alpha_1 + n_1) \dots \Gamma(\alpha_k + n_k)}{\Gamma(\alpha_1 + \dots + \alpha_k + n)} \end{aligned}$$

$$\begin{aligned} P(\psi_n | \psi_1, \dots, \psi_{n-1}) &= \frac{\Gamma(\alpha_1 + n_1) \dots \Gamma(\alpha_k + n_k)}{\Gamma(\alpha_1 + \dots + \alpha_k + n)} \frac{\Gamma(\alpha_1 + \dots + \alpha_k + n - 1)}{\Gamma(\alpha_1 + \tilde{n}_1) \dots \Gamma(\alpha_k + \tilde{n}_k)} \\ &= \frac{\alpha_k + n_k}{\sum \alpha_k + n} \quad \text{if } \psi_n = k. \end{aligned}$$

$$P(\psi_n | \psi_1, \dots, \psi_{n-1}) \propto \alpha_k + n_k \quad \text{if } \psi_n = k$$

Suppose that we can somehow let $K \rightarrow \infty$, yet $\alpha_k = \frac{\alpha}{K}$
 so that $\sum \alpha_k = \alpha$ fixed, then

$$P(\psi_n | \psi_1, \dots, \psi_{n-1}) \propto n_k \quad \text{if } \psi_n = k.$$

there is a remaining probability that $\psi_n \neq \psi_1, \dots, \psi_{n-1}$
 that probability $\rightarrow \frac{\alpha}{\alpha + n}$

How is this related to ~~Dir~~ ^{stick-breaking?} ?

- As $K \rightarrow \infty$, $\pi \rightarrow$ Dirichlet process
- Reorder (π_1, \dots, π_k) in decreasing order then $(\pi_1, \dots, \pi_k) \rightarrow$ stick breaking process

• Now we're ready to state original def of Dirichlet process.

• Stochastic process vs. RV's. ^{real-valued}
Elementary prob. thm : RV's are function $X: \Omega \rightarrow \mathbb{R}$
 Ω : set of events
 $P(X \leq t) = P(\{X(\omega) \leq t\})$.

A stochastic process can be viewed as a dist/measure on space of more complex objects such as functions or measures.
therefore, Random functions or random measures.

• Gaussian process as def dist on $\{X: T \rightarrow \mathbb{R}\}$
is defined as a collection of RV's $\{X(t) : \Omega \rightarrow \mathbb{R}\}_{t \in T}$
s.t. every finite collection of $\{X(t)\}_{t \in S}$ is a multivariate Gaussian
and that they are consistent w/ each other thru marginalization

• Kolmogorov's thm says that then there exists a meaningful dist on the space of function $\{X: T \rightarrow \mathbb{R}\}$ which is called a Gaussian process..

For Gaussian, consistency is obviously satisfied: $(X_1, X_2) \sim N$ then $X_1 \sim N$.

• A probability measure (dist) G is a function that map ~~set~~ ^{a probability space} Ω to $[0, 1]$
 $A \in \Omega$ $G(A) \equiv$ probability $\omega \in A$ under G .
i.e. if $X \sim G$ then $P(X \in A) = G(A)$.

• To define a Random measure ~~by~~ G means the collecting $\{G(A)\}_{A \subset \Omega}$ ^B ~~or~~ collecting RV's.

Def: Let (Ω, \mathcal{F}) a prob. space.
 if G is a Random measure on (Ω, \mathcal{F}) s.t

for any partition (A_1, A_2, \dots, A_k) of Ω , $k \in \mathbb{N}$
 $(G(A_1), G(A_2), \dots, G(A_k)) \sim \text{Dir}(\alpha G_0(A_1), \dots, \alpha G_0(A_k))$


then G is said to be dist accordy to a Dirichlet proc
 G_0 is called a base measure (mean measure)
 α concentrati parameter.

Non sure DP exists due to consistency property of finite dir
 Dir dist: if $(Y_1, \dots, Y_k) \sim \text{Dir}(\alpha_1, \dots, \alpha_k)$, then $(Y_1 + Y_2, \dots, Y_{k-1} + Y_k)$
 $\sim \text{Dir}(\alpha_1 + \alpha_2, \dots, \alpha_{k-1} + \alpha_k)$

Fact: if $G \sim \text{DP}(\alpha, G_0)$
 then $G(A) \sim \text{Beta}(\alpha G_0(A), \alpha(1 - G_0(A)))$

$\rightarrow \begin{cases} E G(A) = \frac{G_0(A)}{\alpha G_0(A) + 1} \\ \text{var } G(A) = \frac{G_0(A)}{\alpha(\alpha + 1)} \end{cases}$

Question: if $\begin{cases} G \sim \text{DP}(\alpha, G_0) \\ \Theta | G \sim G \end{cases}$

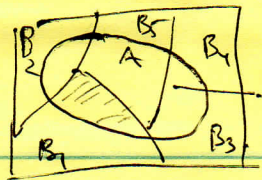


what is the posterior of $[G | \Theta]$?

$\forall A \in \mathcal{F} \quad P(X \in A | G(A)) = G(A) \text{ a.s.}$
 $\Rightarrow P(X \in A) = E G(A) = G_0(A)$

Take a ^{measurable} partition (B_1, \dots, B_k) $\sim \text{Dir}(\alpha G_0(B_1), \dots, \alpha G_0(B_k))$

Thm $[G(B_1), \dots, G(B_k) | X] \sim \text{Dir}(\alpha G_0(B_1) + \delta_{B_1}^{(X)}, \dots)$



$$\begin{aligned}
 & P(X \in A; G(B_1) \leq y_1, \dots, G(B_K) \leq y_K) \\
 &= \sum_{k=1}^K P(X \in B'_k; G(B_1) \leq y_1, \dots, G(B_K) \leq y_K) \\
 &= \sum_{k=1}^K P(X \in B_i) P(G(B_1) \leq y_1, \dots, G(B_K) \leq y_K \mid X \in B'_i) \\
 &= \sum_{k=1}^K G_0(B'_i) \text{Dir}(G(B'_i) + G(B''_i) \leq y_1, \dots \mid X \in B'_i)
 \end{aligned}$$

$$B'_i = A \cap B_i$$

Note that $(G(B'_1), G(B''_1), \dots, G(B'_K), G(B''_K)) \sim \text{Dir}(\alpha G_0, \dots)$

By ~~mult~~ Dir-Mult Conjugacy:

$$\begin{aligned}
 & (G(B'_1), G(B''_1), \dots) \mid X \in B'_i \\
 & \sim \text{Dir}(\alpha G_0(B'_i) + \delta_{B'_i}, \dots)
 \end{aligned}$$

$$= \sum_{k=1}^K G_0(B'_i) \text{Dir}(G(B_1) \leq y_1, \dots, G(B_K) \leq y_K \mid \alpha G_0(B_1) + \delta_{B_1}, \dots, \alpha G_0(B_K) + \delta_{B_K})$$

$$\text{So } P(G(B_1) \leq y_1, \dots, G(B_K) \leq y_K \mid X \in A)$$

$$= \sum_{k=1}^K \frac{G_0(B'_i)}{G_0(A)} P(G(B_1) \leq y_1, \dots, G(B_K) \leq y_K \mid \alpha G_0(B'_i) + \delta_{B'_i}, \dots, \alpha G_0(B_K) + \delta_{B_K})$$

$$\text{if } A \subset B_i \text{ then } P(G(B_1) \leq y_1, \dots, G(B_K) \leq y_K \mid X \in A)$$

$$= P(G(B_1) \leq y_1, \dots, G(B_K) \leq y_K \mid \alpha G_0(B_1) + \delta_{B_1}, \dots)$$

$$\text{Since } (G(B_1), \dots, G(B_K)) \sim \text{Dir}(\alpha G_0(B_1) + \delta_{B_1}, \dots)$$

Schurman

Let β_k Beta (hdd) $\delta_k \stackrel{\text{ind}}{\sim} G_0$

Th β_k

$$\beta_k \beta_k(L_{\beta_k}) \cdot (1 - \beta_k) = \beta_k (1 - \beta_k)$$

then let $G = \sum \beta_k \delta_{G_k}$

Thm $G \sim DP(\alpha, G_0)$

$$\begin{aligned} G &= \beta_1 \delta_{G_1} + (1 - \beta_1) \left[\beta_2 \delta_{G_2} + (1 - \beta_2) \beta_3 \delta_{G_3} + \dots \right] \\ &= \beta_1 \delta_{G_1} + (1 - \beta_1) G' \end{aligned}$$

$G' \stackrel{\text{ind}}{\sim} \beta_k \delta_{G_k}$

So $G \stackrel{\text{dist}}{=} \beta_1 \delta_{G_1} + (1 - \beta_1) G$

let (B_1, \dots, B_k) be a partition

$$P = (G(B_1), \dots, G(B_k))$$

then

$$P = \beta_1 (\delta_{G_1}(B_1), \dots, \delta_{G_1}(B_k)) + (1 - \beta_1) P \quad (*)$$

Can easily check that

$$\text{Dir}(\alpha G_0(B_1), \dots, \alpha G_0(B_k)) \stackrel{\text{dist}}{=} \beta_1 (\delta_{G_1}(B_1), \dots, \delta_{G_1}(B_k)) + (1 - \beta_1) \text{Dir}(\alpha G_0(B_1), \dots, \alpha G_0(B_k))$$

if $G \in B_i$ then $\beta_1 (1, 0, \dots, 0) + (1 - \beta_1) \text{Dir}(\alpha G_0(B_1), \dots)$

$$\sum_{j=1}^k P(G_j \in B_j) \text{Dir}(\alpha G_0 + \delta_{e_j}) = \text{Dir}(\alpha G_0)$$

next Lemma N, U, W RV's, $W \in [-1, 1]$

U, V taking value in some vector space

and $\begin{cases} V \stackrel{\text{dist}}{=} U + WV \\ P(|W|=1) \neq 1 \end{cases}$ then V is unique.

if $V \stackrel{\text{dist}}{\neq} V'$ $V_{n+1} = U_n + W_n V_n$
 $V'_{n+1} = U_n + W_n V'_n$

$\Rightarrow |V_{n+1} - V'_{n+1}| = |W_n| |V_n - V'_n| \rightarrow 0$ w.p.1.

This then proves automatically that \mathbb{P} distributed Random measures are discrete w.p.1.

Alternative proof of discreteness

$G \sim DP(\alpha, G_0)$

$X | G \sim G$

then $G | X \sim DP(\alpha G_0 + \delta_X)$.

$G | X_1, \dots, X_n \sim DP(\alpha G_0 + \sum_{i=1}^n \delta_{X_i})$

$DP(\alpha + n, \frac{\alpha G_0}{\alpha + n} + \sum_{i=1}^n \frac{1}{\alpha + n} \delta_{X_i})$.

as $n \rightarrow \infty$: $\begin{cases} \alpha + n \text{ increments} \rightarrow \infty \\ \text{base measure} \rightarrow \frac{1}{n} \sum_{i=1}^n \delta_{X_i} \end{cases}$