Bayesian Nonparametrics (BNP)

Chapter 7 by David B. Dunson

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Textbook

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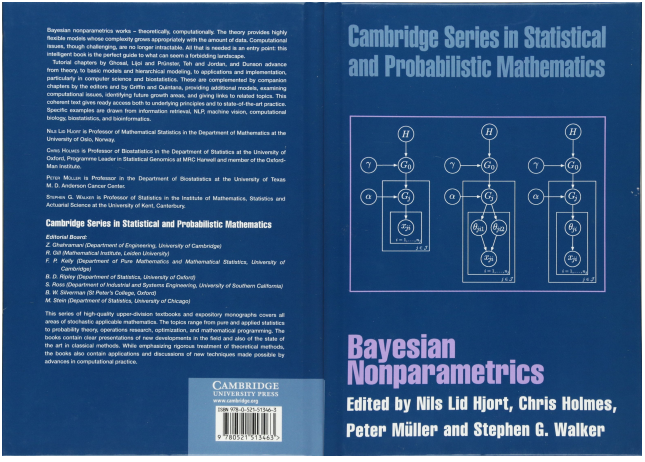


Preliminary

Real Analysis: Lebesgue measure

Probability Theory: Borel σ-field, probability space $(\Omega, \mathcal{F}, P)$

Stochastic Process: e.g., Chinese restaurant process, Indian buffet process

Experimental Design: linear mixed model

Generalized Linear Model: generalized estimating equations, generalized least squares

Bayesian Statistics: exchangeability, mixtures of g-priors, Markov chain Monte Carlo

Machine Learning: clustering, Gaussian mixture model

Nonparametric Bayes

Bayes' theorem: Posterior $\propto$ Likelihood $\times$ Prior

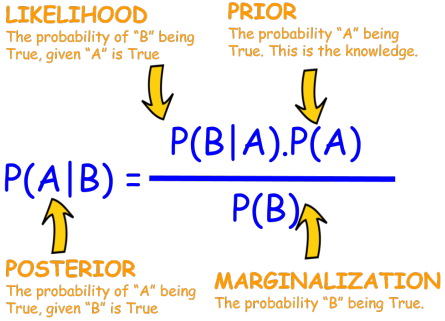


Image: Towards Data Science

Bayesian parametric model: A - parameters; B - data.
Bayesian nonparametric model: unbounded / growing / **infinite** number of parameters.

Repeated-Measures Design

- Longitudinal data: collected on the same subjects over time.
- Clustered data: measurements made on all units within a cluster in Eq. 1 & 2.

  Intraclass correlation $\rho = \dfrac{g}{g + \sigma^2}$

  - proportion of total variance due to within-cluster variance;
  - how strongly units within same cluster resemble each other.

$$\mathcal{M}_1: \quad y_{ij} = \mu_i + \epsilon_{ij}, \quad \epsilon_{ij} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \tag{1}$$

where y_{ij} is the jth observation within subject i,
μ_i is a subject-specific mean,
ϵ_{ij} is an observation-specific residual,
σ is the within-subject standard deviation,
g is the between-subject variance on p. 7,
for $j = 1, \cdots, n_i$ and $i = 1, \cdots, n$.

Same Mixed Model but Different Designs

- Clustered data (Dobson & Barnett, 2018, p. 259; Dunson, 2010, p. 224)

  e.g., the income of the jth household in the randomly selected council area i
  e.g., the weight of the jth piglet in the randomly selected litter i

$$\begin{aligned} \mathcal{M}_1\text{:} \quad & y_{ij} = \mu + b_i + \epsilon_{ij} \\ \text{versus} \quad \mathcal{M}_0\text{:} \quad & y_{ij} = \mu + \epsilon_{ij} \end{aligned}$$

- One-way within-subject data (Rouder et al., 2012 & 2017)

  e.g., the response time of the ith subject for the jth Stroop task

$$\begin{aligned} \mathcal{M}_1\text{:} \quad & y_{ij} = \mu + b_i + t_j + \epsilon_{ij} \\ \text{versus} \quad \mathcal{M}_0\text{:} \quad & y_{ij} = \mu + b_i + \epsilon_{ij} \end{aligned}$$

Bayesian Parametric Modeling

$$\mathcal{M}_1: \quad y_{ij} = \mu_i + \epsilon_{ij}, \quad \epsilon_{ij} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \tag{1}$$

$$\mu_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, g) \tag{2}$$

$$\text{or} \quad \mu_i = \underbrace{\mu}_{\text{fixed}} + \underbrace{b_i}_{\text{random effects}}, \qquad b_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, g) \tag{3}$$

BNP Motivation

The normal distribution has light tails and does **not** allow some subjects to be very different from other subjects or to have groups of subjects that cluster close together. Hence, outlying subjects tend to have their means **over-shrunk** towards the population mean, and the data from such subjects may be overly-influential in estimation of the overall mean μ.

The t-distribution has heavier tails, but it still has a very restrictive unimodal and symmetric shape.

Bayesian Nonparametric Modeling

$$\mathcal{M}_1: \quad y_{ij} = \mu_i + \epsilon_{ij}, \quad \epsilon_{ij} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \tag{1}$$

$$\mu_i \overset{\text{i.i.d.}}{\sim} P \tag{4}$$

$$P \sim DP(P_0, \alpha) \tag{5}$$

Choose a **Dirichlet process** (DP) prior for P.

P corresponds to a distribution function, or more formally, a random probability measure.

- Eq. 5 allows P to be an unknown distribution.
- P_0 is a fixed baseline probability measure (the expected value of the process), corresponding to one's best guess for P *a priori*,
  e.g., P_0 is a normal distribution with the normal-inverse gamma hyperpriors.
- α is the concentration parameter ($\alpha > 0$),
  characterizing prior precision and clustering (expressing confidence in P guess),
  e.g., $\alpha \sim \text{Gamma}(1, 1)$, a gamma hyperprior.

Hierarchical Dirichlet Process

Chinese restaurant *franchise* (Teh et al., 2006)

$$\mu_i \mid P_i \sim P_i$$

$$P_i \mid P_0, \alpha_i \sim \mathit{DP}(P_0, \alpha_i)$$

$$P_0 \mid H, \alpha \sim \mathit{DP}(H, \alpha)$$

mixed model $\neq$ mixture model

Dirichlet Distribution

The Dirichlet distribution, $\mathrm{Dir}(\boldsymbol{\alpha})$, is a multivariate generalization of the beta distribution for $K \geqslant 2$. The PDF is

$$f(x_1, \cdots, x_K; \alpha_1, \cdots, \alpha_K) = \frac{1}{\mathrm{B}(\boldsymbol{\alpha})} \prod_{i=1}^{K} x_i^{\alpha_i - 1}, \tag{6}$$

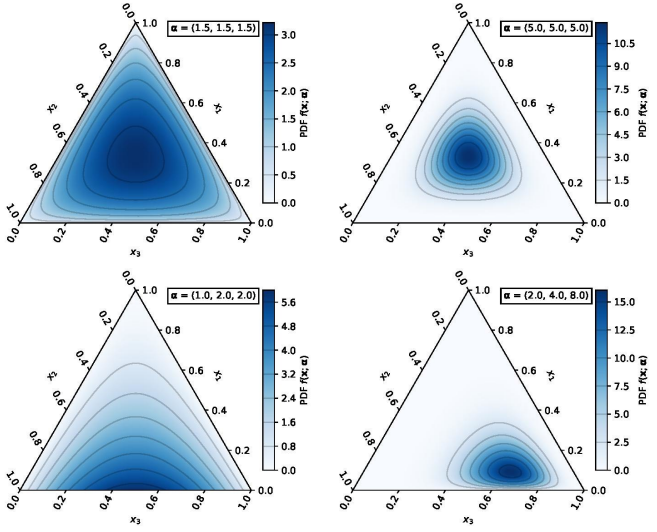
where $\mathrm{B}(\boldsymbol{\alpha}) = \dfrac{\prod_{i=1}^{K} \Gamma(\alpha_i)}{\Gamma(\alpha_0)}$,

$$\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_K), \quad \alpha_0 = \sum_{i=1}^{K} \alpha_i \tag{7}$$

$$\sum_{i=1}^{K} x_i = 1 \text{ and } x_i \geqslant 0, \ \alpha_i > 0 \text{ for } i = 1, \cdots, K.$$

- If $\alpha_1 = \cdots = \alpha_K = \alpha$, the Dirichlet distribution will be symmetric.
- When $\alpha = 1$, it is a uniform distribution over the open standard $(K-1)$-simplex.

Simplex



Source: Wikipedia

R Scripts

```
options(digits=3); set.seed(277)
# LaplacesDemon::rdirichlet()
(pis <- gtools::rdirichlet(n=3, #number of random vectors to generate
                           alpha=rep(1,5)))
#         [,1]   [,2]   [,3]    [,4]   [,5]
# [1,] 0.35982 0.2053 0.0148 0.07106 0.3490
# [2,] 0.00204 0.2274 0.6151 0.00293 0.1525
# [3,] 0.61949 0.0075 0.2448 0.06353 0.0647

rowSums(pis) # 1 1 1
gtools::rdirichlet(3, rep(1000,5))
#       [,1]  [,2]  [,3]  [,4]  [,5]
# [1,] 0.208 0.200 0.207 0.193 0.193
# [2,] 0.190 0.210 0.199 0.199 0.203
# [3,] 0.194 0.207 0.195 0.206 0.198
```

$\text{Dir}(\boldsymbol{\alpha})$ is the canonical Bayesian distribution for the parameter estimates of a multinomial distribution.

$z_i \mid \boldsymbol{\pi} \sim \text{Cat}(\boldsymbol{\pi})$. A Distribution over distributions.

Relation to the Gamma Distribution

For K independently distributed gamma distributions,

$$Y_i \overset{\text{ind.}}{\sim} \text{Gamma}(\alpha_i, \beta) \quad \text{for } i = 1, \cdots, K,$$

it can be proved that the sum is also a gamma distribution,

$$Y = \sum_{i=1}^{K} Y_i \sim \text{Gamma}\left(\alpha_0, \beta\right). \tag{8}$$

Then, the K-dimensional Dirichlet distributed random vector is

$$\boldsymbol{X} = (X_1, \cdots, X_K) = \left(\frac{Y_1}{Y}, \cdots, \frac{Y_K}{Y}\right) \sim \text{Dir}(\boldsymbol{\alpha}). \tag{9}$$

$\text{Cov}(X_i, X_j) = \dfrac{-\alpha_i \alpha_j}{\alpha_0^2(\alpha_0 + 1)}$ for $i \neq j$, not independent.

The marginal distributions are $X_i \sim \text{Beta}(\alpha_i, \alpha_0 - \alpha_i)$. Exponential family.

Properties

If $(X_1, \cdots, X_K) \sim \text{Dir}(\alpha_1, \cdots, \alpha_K)$, $\quad \mathbb{E}[X_i] = \alpha_i/\alpha_0$ and $\text{Var}(X_i) = \alpha_i(\alpha_0 - \alpha_i)/(\alpha_0^2(\alpha_0 + 1))$

- Collapsing

then $(X_1 + X_2,\ X_3, \cdots, X_K) \sim \text{Dir}(\alpha_1 + \alpha_2,\ \alpha_3, \cdots, \alpha_K)$.

- Splitting

$(\varphi_1, \cdots, \varphi_N) \sim \text{Dir}(\alpha_1 w_1, \cdots, \alpha_1 w_N)$, and $\sum_{j=1}^{N} w_j = 1$,

then $(X_1\varphi_1, \cdots, X_1\varphi_N,\ X_2, \cdots, X_K) \sim \text{Dir}(\alpha_1 w_1, \cdots, \alpha_1 w_N,\ \alpha_2, \cdots, \alpha_K)$.

- Renormalization

then $(X_2/S, \cdots, X_K/S) \sim \text{Dir}(\alpha_2, \cdots, \alpha_K)$, where $S = \sum_{i=2}^{K} X_i$.

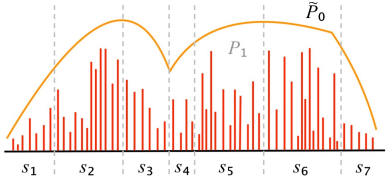
Transitioning to the Dirichlet Process

For any finite partition $S_1, \cdots, S_K$ of the measurable set S, $\left(\sum_{i=1}^{K} P_0(S_i) = 1\right)$,

$P \sim DP(P_0, \alpha)$,

$\Updownarrow$

$(P(S_1), \cdots, P(S_K)) \sim \text{Dir}(\alpha P_0(S_1), \cdots, \alpha P_0(S_K))$.



Recall marginal betas.

Note that $\mathbb{E}[P(S_i)] = P_0(S_i)$ and $\text{Var}(P(S_i)) = \dfrac{P_0(S_i)(1 - P_0(S_i))}{\alpha + 1}$.

α determines the variance of the random probability measure.

Dirichlet Process

The infinite-dimensional generalization of the Dirichlet distribution is the Dirichlet process $DP(P_0, \alpha)$. View 1

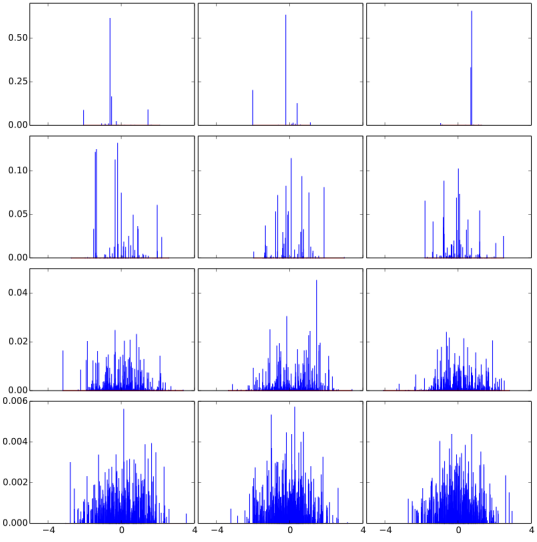
- Even if P_0 is continuous, the distributions drawn from the Dirichlet process are almost surely **discrete**.
- α specifies how strong this discretization is.
  - As $\alpha \to 0$, the realizations are all concentrated at a single value.
  - As $\alpha \to +\infty$, the realizations become continuous.

$DP(P_0, \alpha)$ is often used in Bayesian inference to describe the prior knowledge about the distribution of random variables — how likely it is that the random variables are distributed according to one or another particular distribution.

Example: $DP(\mathcal{N}(0,1),\alpha)$

$\alpha = 1,\ 10,\ 100,\ 1,000$ from top to bottom.

Each row contains three repetitions of the same process.



Source: Wikipedia

Why *DP*?

In continuous measures, the probability of picking the **same** value twice is zero,

whereas in discrete measures, it is non-zero.

Posterior: Spike-and-Slab

$$m_i \overset{\text{i.i.d.}}{\sim} P \qquad \text{for } i = 1, \cdots, n$$
$$P \sim DP(P_0, \alpha)$$

Given observed data and a DP prior, we update our beliefs about the underlying distribution based on that data.
The posterior of P is

$$P \mid \boldsymbol{m} \sim DP\left(\frac{\alpha \overset{\text{PDF}}{P_0} + \overset{\text{PMF}}{\sum_{i=1}^{n} \delta_{m_i}}}{\alpha + n},\ \alpha + n \right). \tag{10}$$

The base probability measure for the posterior DP can involve a mix of the continuous distribution (the "slab") and the point masses (the "spikes").

See also the Bayesian variable selection.

Predictive Distribution

A new data point can join either an existing or a new cluster k.

$$
\begin{aligned}
&\mathbb{P}(X_{n+1} = \theta_k \mid X_1, \cdots, X_n) \\
=&\int \mathbb{P}(X_{n+1} = \theta_k \mid \pi) \cdot \mathbb{P}(\pi \mid X_1, \cdots, X_n)\, \mathrm{d}\pi \\
=&\mathbb{E}_{\mathsf{Dir}(n_1, \cdots, n_K, \alpha)}[\pi_k] \qquad (11) \\
=&\begin{cases} \dfrac{n_k}{\alpha + n}, & \text{if } k \leqslant K, \\ \dfrac{\alpha}{\alpha + n}, & \text{for a new cluster,} \end{cases}
\end{aligned}
$$

where n_k is the number of times that $X_i = \theta_k$ for $i = 1, \cdots, n$, and K is the total number of existing clusters.

Chinese Restaurant Process (CRP)

Jim Pitman and Lester E. Dubins, San Francisco

Metaphorical Setting: View 2

Imagine a restaurant with an infinite number of tables, each capable of seating an infinite number of customers. The first customer sits at the first table.

Each subsequent customer decides where to sit according to certain probabilistic rules.

The probability of the ith customer ($i \geqslant 2$) sitting at

- an exisiting table k is $\dfrac{n_k}{\alpha + i - 1}$,
- a new table is $\dfrac{\alpha}{\alpha + i - 1}$.

Recall Eq. 4, $\mathbb{P}(\mathcal{H}_0 \colon \mu_h = \mu_l) = \dfrac{1}{\alpha + 1}$.

Stick-Breaking Representation

Question: How do we draw a random distribution P from the Dirichlet process?

View 3

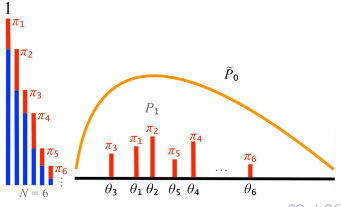
$P \sim DP(P_0, \alpha)$ is equivalent to assigning weights to point masses at *atoms* θ_h,

$$P = \underset{\text{PMF}}{p(\theta)} = \sum_{h=1}^{\infty} \pi_h \cdot \delta_{\theta_h}(\theta), \quad \theta_h \overset{\text{i.i.d.}}{\sim} P_0, \tag{12}$$

where $\pi_1 = V_1$ and $\pi_h = V_h \prod_{l<h}(1 - V_l)$ are probability weights that are formulated from a stick-breaking process with $V_h \overset{\text{i.i.d.}}{\sim} \text{Beta}(1, \alpha)$ for $h = 1, \cdots, \infty$,

and $\delta_{\theta_h}(\cdot)$ is the indicator function $\delta_{\theta_h}(\theta_h) = 1$, otherwise 0.

In practice, we choose some N to truncate the series.



R Scripts (continued)

```
stick_breaking_process <- function(N, alpha) {
  #' Input -
  #' N:       number of weights (stick-breaks)
  #' alpha:   concentration
  #' Output - a vector of weights
  V <- rbeta(N, 1, alpha)
  V * c(1, cumprod(1-V))[1:N]
}

N <- 1000; alpha <- 100; set.seed(277)
# Each random number from the base measure N(0,1) is
#  replicated a number of times corresponding to its weight.
draws <- rep(rnorm(N),
             round(stick_breaking_process(N, alpha) * 10000))

hist(draws, prob=T, col="white", yaxt="n", ylab="", xlab=expression(theta),
     main="Random Distribution From the Dirichlet Process")
lines(density(draws), col="red", lwd=2)
```

"The rich get richer" (Shelley, 1821): Frequently sampled values in the past are more likely to be picked again.

Modified Pólya Urn Scheme

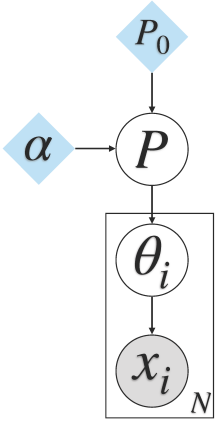
Blackwell-MacQueen Sampling Scheme

View 4

1. An urn contains balls of different colors, ●●●●●●⋯, e.g., α black balls ●.
2. A ball is drawn randomly from the urn.
3. **Reinforcement**:
   If the drawn ball is black, place ● back along with a (new) non-black ball, e.g., ●.
   Otherwise, place it back with an additional ball of the same color, e.g., ● in the urn.
4. Repeat Steps 2 and 3.

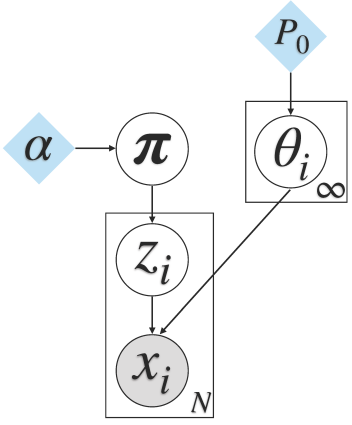
The resulting distribution over generated colors
is the same as P over tables in the CRP, $P \sim DP(P_0, \alpha)$.

Graphical Models



The Pólya Urn Scheme

$\equiv$



The Stick-Breaking Representation

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Thank you.

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