Prior-Driven Cluster Allocation in Bayesian Mixture Models

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JSM 2020

August 03, 2020

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Introduction

Clustering is one of the canonical data analysis goal in statistics

- **Distance based methods**: distance metric between data points
- **Model-based clustering**: rely on discrete mixture models

Bayesian perspective : allow to incorporate prior information

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What if, we have prior information on the clustering itself?

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What if, we have prior information on the clustering itself?

Motivating application - **Birth defects data**

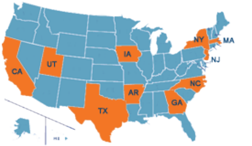
- Relate exposure factors to the development risk of a defect
- **Prior information** available (biology/expert's judgments)

➔ We aim to provide methods to facilitate data-adaptive clustering, both using **information in the data** and **external knowledge**.

National Birth Defect Prevention Study

- **Population-based case-control study**
  - ➔300 controls/100 cases per year since 1997
  - ➔monthly n. of controls $\propto$ n. of births previous year
- **Cases** (37 major birth defect)
  - ➔Birth defects surveillance system
  - $+$clinical genetist review
  - ➔Cases with known etiology were excluded
- **Controls**
  - ➔Non-malformed live birth
  - ➔Birth certificates or hospital delivery records
- **Data collection**
  - ➔CATI (English/Spanish) within 24 months

national • birth • defects • prevention • study



http://www.nbdps.org/

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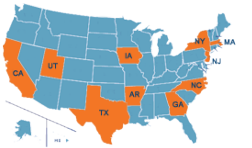

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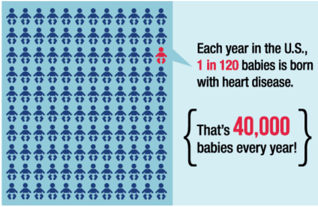
We focus on the **Congenital Heart Defects** (**CDH**) which are problems in the structure of the heart that are present at birth.

Congenital Heart Defects



Clinical importance

priority in public health

→most frequent class of defects

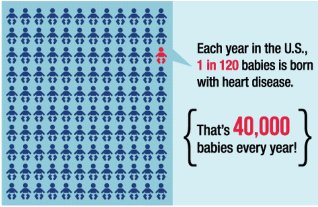
→high impact on pediatric mortality

Statistical relevance: challenge in birth defects modeling

→Most defects are too rare for individual study

→Difficult to determine how best to group birth defects

Congenital Heart Defects



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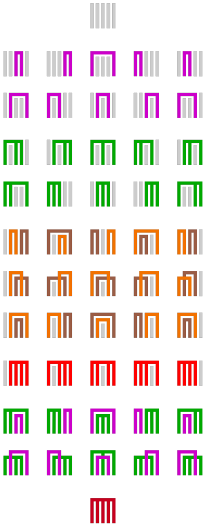
Experts have provided a **mechanistic classification** of the defects

- → relies on biological knowledge and embryologic development
- → **translates in a prior guess c_0 for the clustering**

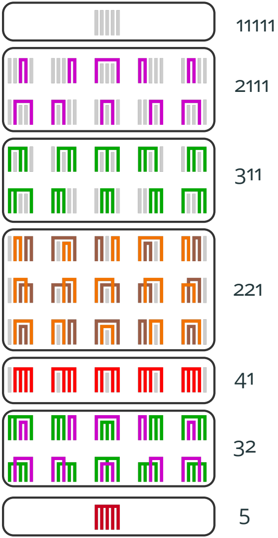
Set partitions



A **set partition** $\boldsymbol{c}$ of an integer $[n]$ is a collection of non-empty disjoint subsets $\{B_1, B_2, \ldots, B_K\}$ such that $\cup_i^K B_i = [n]$

- Number of partitions of $[n]$ into k blocks
  →Stirling numbers $S(n, k)$
- Total number of set partitions
  →Bell number $\mathcal{B}_n = \sum_{k=1}^{n} S(n, k)$

Set partitions



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- Total number of set partitions
  →Bell number $\mathcal{B}_n = \sum_{k=1}^{n} S(n, k)$
- **Configuration** $\boldsymbol{\lambda} = \{|B_1|, \ldots, |B_K|\}$
  →sequence of block cardinalities
  →individuate an **integer partition**, a set of positive integers $\{\lambda_1, \ldots, \lambda_K\}$ such that $\sum_{i=1}^{K} \lambda_i = n$

Modeling birth defects

- $i = 1, \ldots, N$ heart defects, $j = 1, \ldots, n_i$ observations
- $y_{ij} = 1$ if observation j has the b.d. i while $y_{ij} = 0$ is a control
- $\mathbf{x}_{ij}^T = (x_{ij1}, \ldots, x_{ijp})$ observed values for p dichotomous variables

Grouped logistic regression

$$
\begin{aligned}
y_{ij} &\sim Ber(\pi_{ij}) \qquad \text{logit}(\pi_{ij}) = \alpha_i + \mathbf{x}_{ij}^T \boldsymbol{\beta}_{c_i}, \quad j = 1, \ldots, n_i, \\
\alpha_i &\sim \mathcal{N}(a_0, \tau_0^{-1}) \qquad \boldsymbol{\beta}_{c_i} | \boldsymbol{c} \sim \mathcal{N}_p(\mathbf{b}, \mathbf{Q}) \quad i = 1, \ldots, N,
\end{aligned}
$$

Bayesian framework: assign a prior probability $p(\boldsymbol{c})$

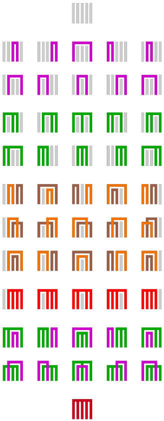
➔*Exchangeable Partition Probability Function* (EPPF)

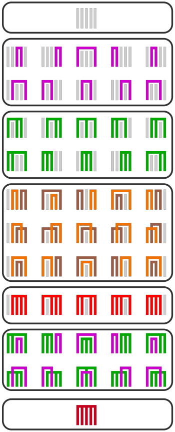
Uniform distribution

$p(\boldsymbol{c}) \propto 1/\mathcal{B}_N$

Dirichlet Process: $p(\boldsymbol{c}) \propto \prod_{i=1}^{K}(|B_i| - 1)!$

Pitman-Yor Process: $p(\boldsymbol{c}) \propto \prod_{i=1}^{K}(1-\sigma)_{|B_i|}$





How to account for c_0?

Base idea: penalize a baseline EPPF in order to center the prior distribution on the given partition $\boldsymbol{c}_0$

$$p(\boldsymbol{c}|\boldsymbol{c}_0, \psi) \propto p_0(\boldsymbol{c}) \exp\{-\psi d(\boldsymbol{c}, \boldsymbol{c}_0)\} \tag{1}$$

- $p_0(\boldsymbol{c})$ indicates a **baseline distribution** (EPPF) on Π_N
- $d(\boldsymbol{c}, \boldsymbol{c}_0)$ a suitable **distance** between partitions
  ➔ideally a metric on the set partitions lattice
- ψ **penalization parameter** controlling for the centering
  ➔ $\psi = 0 \quad p(\boldsymbol{c}|\boldsymbol{c}_0, \psi) \to p_0(\boldsymbol{c})$
  ➔ $\psi \to \infty \quad p(\boldsymbol{c}|\boldsymbol{c}_0, \psi) = \delta_{\boldsymbol{c}_0}$

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Choice of the distance ➔ Variation of information [Meila (2007)]

- $\text{VI}(\boldsymbol{c}, \boldsymbol{c}') = -H(\boldsymbol{c}) - H(\boldsymbol{c}') + 2H(\boldsymbol{c} \wedge \boldsymbol{c}')$
- $H(\cdot)$ information entropy
- metric on set partition lattice

Centered Partition Processes

Define sets of partitions with distance δ_l from $\boldsymbol{c}_0$ and configuration $\boldsymbol{\lambda}_m$

$$s_{lm}(\boldsymbol{c}_0) = \{\boldsymbol{c} \in \Pi_N : d(\boldsymbol{c}, \boldsymbol{c}_0) = \delta_l, \boldsymbol{\Lambda}(\boldsymbol{c}) = \boldsymbol{\lambda}_m\}$$

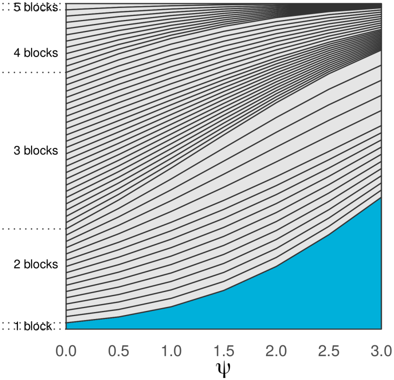
for $l = 0, \ldots, L$ and $m = 1, \ldots, M$.

Centered Partition Processes - analytic form

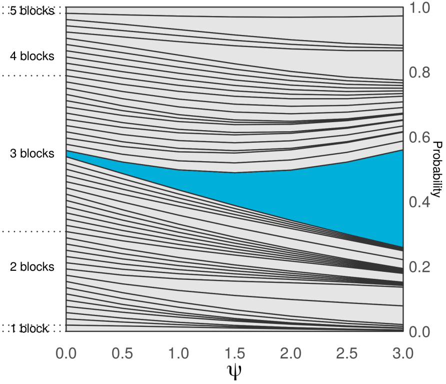
$$p(\boldsymbol{c}|\boldsymbol{c}_0, \psi) = \frac{g(\boldsymbol{\lambda}_m)e^{-\psi\delta_l}}{\sum_{u=0}^{L}\sum_{v=1}^{M} |s_{uv}(\boldsymbol{c}_0)| g(\boldsymbol{\lambda}_v) e^{-\psi\delta_u}}, \quad \text{for } \boldsymbol{c} \in s_{lm}(\boldsymbol{c}_0)$$

- $g(\cdot)$ function of the configuration $\boldsymbol{\Lambda}(\boldsymbol{c})$
  → e.g. Uniform $g(\boldsymbol{\Lambda}(\boldsymbol{c})) = 1$, DP $g(\boldsymbol{\Lambda}(\boldsymbol{c})) = \alpha^K \prod_{j=1}^{K} \Gamma(\lambda_j)$
- $|\cdot|$ cardinality of the set $s_{lm}(\boldsymbol{c}_0)$, not analytically tractable
  → but can nonetheless be used in Bayesian models relying on Monte Carlo methods

CP Process - Uniform EPPF

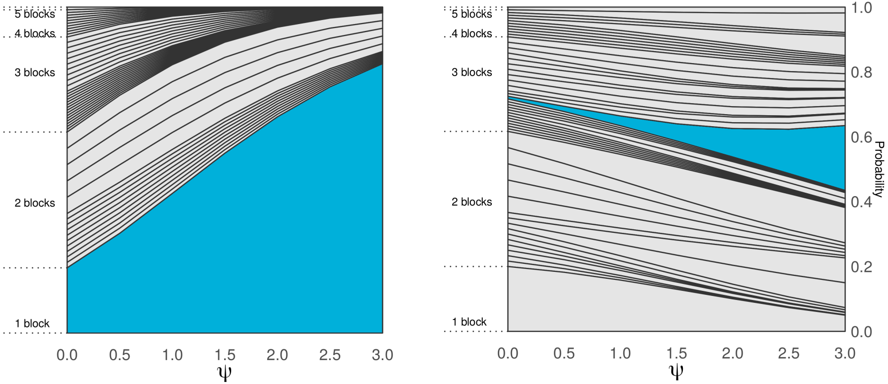


$$c_0 = \{1, 2, 3, 4, 5\}$$



$$c_0 = \{1, 2\}\{3, 4\}\{5\}$$

CP Process - DP EPPF ($\alpha = 1$)



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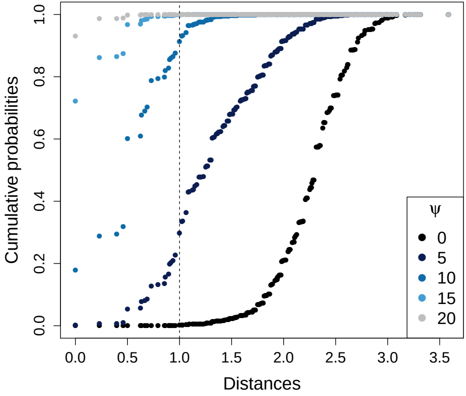
Prior calibration

We consider to estimate the distribution of **distance** $\delta \in \{\delta_l\}_{l=0}^{L}$

$$p(\delta = \delta_l) = \frac{\sum_{m=1}^{M} n_{lm} g(\boldsymbol{\lambda}_m) e^{-\psi\delta_l}}{\sum_{u=0}^{L} \sum_{v=1}^{M} n_{uv} g(\boldsymbol{\lambda}_v) e^{-\psi\delta_u}}$$

- **Monte Carlo procedure**
  ➔ uniform sampler on the set partition space Π_N [Stam (1983)]
- **Deterministic local search**
  ➔ for small values of the distance $\delta \in \{\delta_0, \ldots, \delta_{L^*}\}$
  ➔ greedy search algorithm



Modeling birth defects

$N = 26$ birth defects, $4,047$ cases, $8,125$ controls, 90 potential risk factors

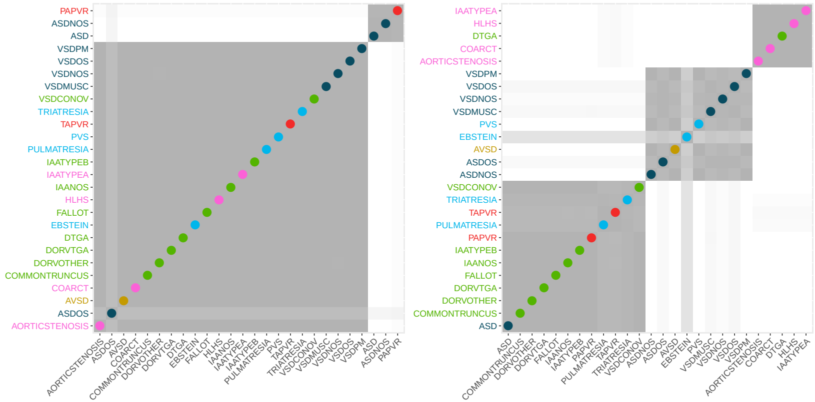
$$y_{ij} \sim Ber(\pi_{ij}) \qquad \text{logit}(\pi_{ij}) = \alpha_i + \mathbf{x}_{ij}^T \boldsymbol{\beta}_{c_i}, \quad j = 1, \ldots, n_i,$$
$$\alpha_i \sim \mathcal{N}(a_0, \tau_0^{-1}) \qquad \boldsymbol{\beta}_{c_i} | \boldsymbol{c} \sim \mathcal{N}_p(\mathbf{b}, \mathbf{Q}) \quad i = 1, \ldots, N,$$
$$p(\boldsymbol{c}) \sim CP(\boldsymbol{c}_0, \psi, p_0(\boldsymbol{c})) \qquad p_0(\boldsymbol{c}) \propto \alpha^K \prod_{k=1}^{K} (\lambda_k - 1)!$$

from the prior calibration: $\psi = 40$ (90% partitions with $d = 0.8$ ($d_{max} = 4.70$)

Posterior estimation (MCMC)

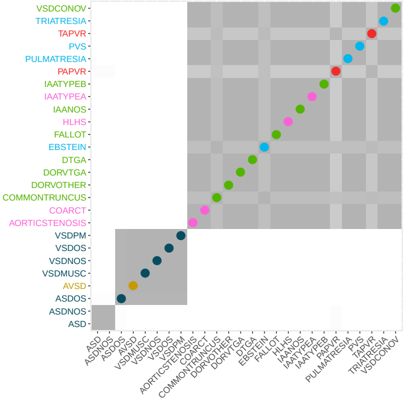
- A **Polya-gamma data augmentation** for Bayesian logistic regression, introducing latent variables $\omega_i^{(j)} \sim PG(1, \alpha^{(j)} + \mathbf{x}_i^{(j)T} \boldsymbol{\beta}^{c_j})$
- Class allocation step involving prior penalization easily adapt marginal sampling for DP process

Clustering results

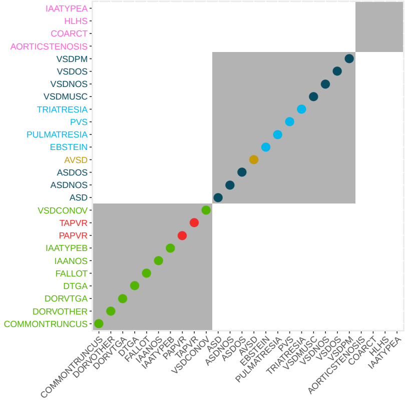


(a) ψ = 0, VI$(\hat{\boldsymbol{c}}, \boldsymbol{c}_0) = 2.43$ **(b)** ψ = 40, VI$(\hat{\boldsymbol{c}}, \boldsymbol{c}_0) = 1.78$

Clustering results

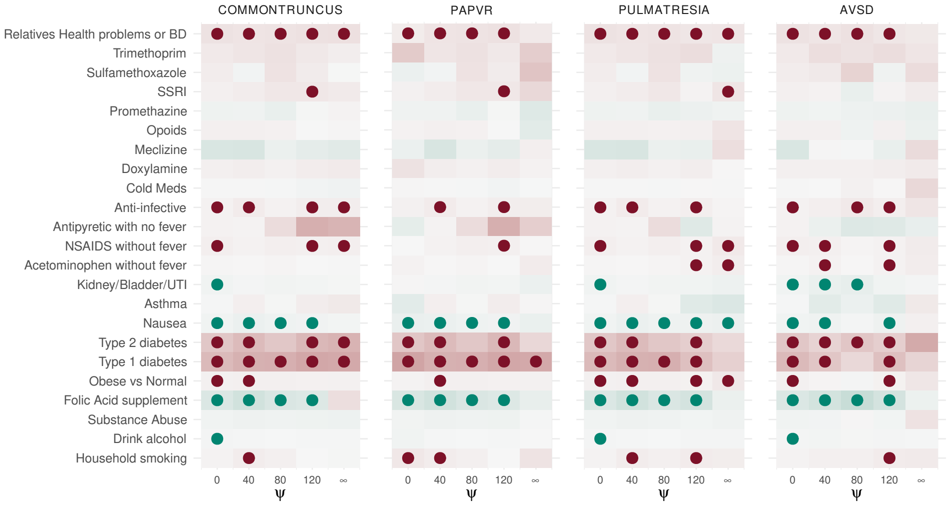


(c) ψ = 80, VI$(\hat{\boldsymbol{c}}, \boldsymbol{c}_0) = 1.65$



(d) ψ = 120, VI$(\hat{\boldsymbol{c}}, \boldsymbol{c}_0) = 0.86$

Exposure effects



Future work

Data analysis

- Variable selection in order to account for shared effects.
- Inclusion of information favoring relation between specific outcomes and exposure factors.

Methodology

- Building prediction rules for new observations/clusters.
- Formalize inclusion of partial information, number/sizes of clusters.

Software

- Provide sampling methods via NIMBLE

Thanks!

Centered Partition Processes: Informative Priors for Clustering.
Paganin S., Herring A. H., Olshan A. F. & Dunson B. D. (2020)
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salleuska

`https://salleuska.github.io/`

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