An introduction to mixture modelling for unsupervised clustering

Mini-tutorial

Nicole M White

Australian Centre for Health Services Innovation (AusHSI)
Queensland University of Technology

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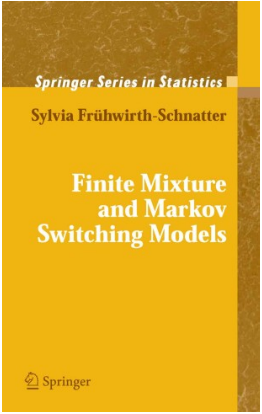
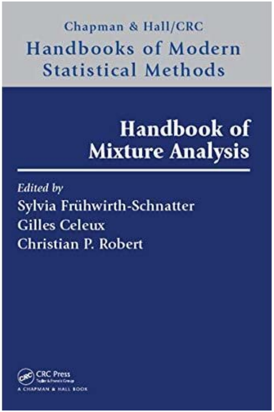
Further reading

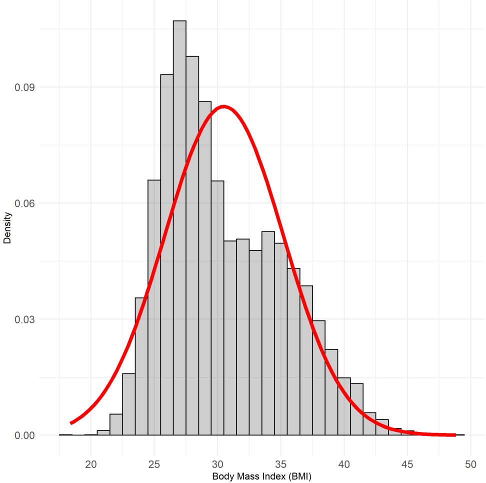




https://github.com/nicolemwhite/anzsc-mixture-modelling

A motivating example

Distribution of body mass index (BMI) for 10,000 participants.



A motivating example

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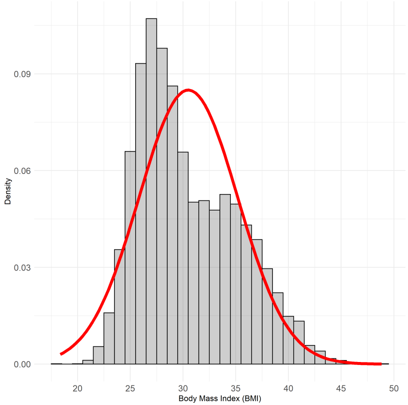
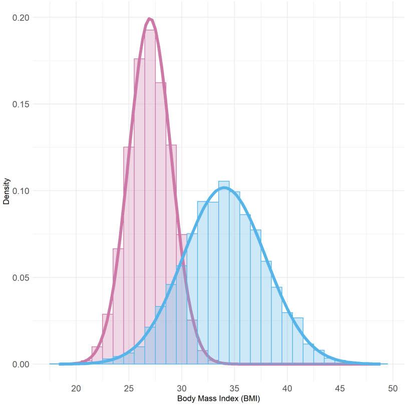
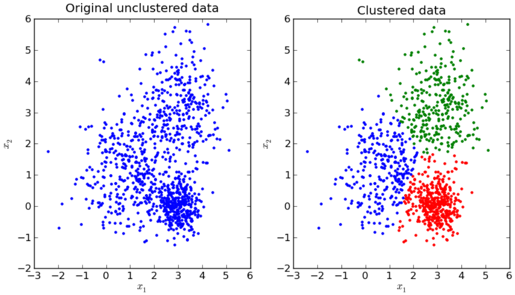




Defining clustering

Unsupervised clustering $\leftrightarrow$ Identifying subgroups

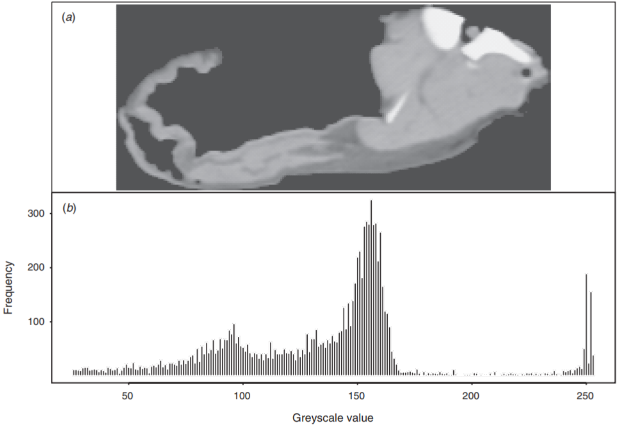


Common approaches:

- Hierarchical clustering, K-means
- Mixture models

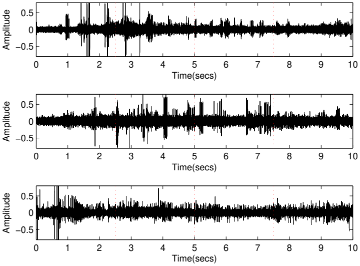
Image source: `https://tinyurl.com/59dbx8u7`

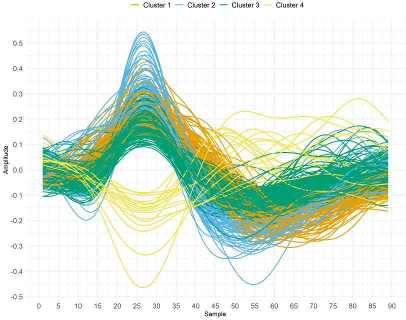
Examples of clustering using mixture models: Image classification



Alston et al (2005) DOI: 10.1071/AR04211

Examples of clustering using mixture models: Spike sorting





Mixture model ingredients

Data are drawn from a *convex combination of components* For K groups/clusters:

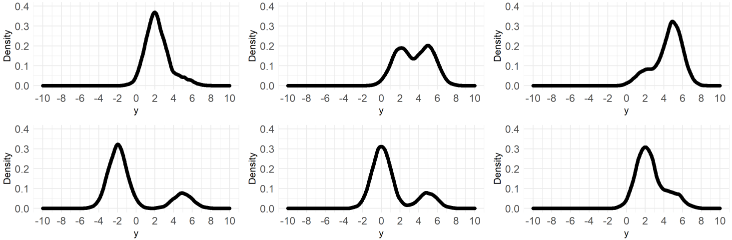
$$
\begin{aligned}
p(y) &= \eta_1 f(y|\boldsymbol{\theta}_1) + \ldots + \eta_K f(y|\boldsymbol{\theta}_K) \\
&= \sum_{k=1}^{K} \eta_k f(y|\boldsymbol{\theta}_k)
\end{aligned}
$$

Unknown parameters: $\boldsymbol{\nu} = (\boldsymbol{\eta}, \boldsymbol{\theta})$

- $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_K)$: Mixture weights; $\sum_{k=1}^{K} \eta_k = 1$
- $f(y|\boldsymbol{\theta}_k)$: k^{th} Mixture component; same parametric family

A simple 2-component mixture model

$$y_i \sim \eta_1 \mathcal{N}(\mu_1, 1) + \eta_2 \mathcal{N}(\mu_2, 1)$$



Mixture model examples

General formulation:

$$p(y_i) = \sum_{k=1}^{K} \eta_k f(y_i|\boldsymbol{\theta}_k)$$

Latent class analysis (J items)

$$f(\mathrm{y}_i|\boldsymbol{\theta}_k) = \prod_{j=1}^{J} f(y_{ij}|\theta_{jk})$$

Latent class regression: $\eta_k \to \eta_k(\mathrm{x}_i)$

$$\eta_k(\mathrm{x}_i) = \frac{exp\left(\mathrm{x}_i^T \beta_k\right)}{\sum_{l=1}^{K} exp\left(\mathrm{x}_i^T \beta_l\right)}$$

Mixture model examples

Focus of mini-tutorial: cross-sectional data

- Finite mixture model
- Dirichlet Process mixture model
- Profile regression

Bayesian approaches to inference: Markov chain Monte Carlo (MCMC)

1. Finite mixture models
2. Dirichlet Process Mixture models
3. Profile regression

Finite mixture model: Setup

Assume:

- K is fixed *a priori*
- Each observation has a probability of belonging to components $1, \ldots, K$

Likelihood for $\boldsymbol{y} = (y_1, \ldots, y_n)$

$$p(\boldsymbol{y}) = \prod_{i=1}^{n} \sum_{k=1}^{K} \eta_k f(y_i | \boldsymbol{\theta}_k)$$

Aim is to learn $\boldsymbol{\nu} = (\boldsymbol{\theta}_{1,\ldots,K}, \boldsymbol{\eta}_{1,\ldots,K})$

Finite Mixture Model: Setup

Likelihood:

$$p(\boldsymbol{y}|\boldsymbol{\nu}) = \prod_{i=1}^{n} \sum_{k=1}^{K} \eta_k f(y_i|\boldsymbol{\theta}_k)$$

Priors:

$$(\eta_1, \ldots, \eta_K) \sim \mathcal{D}(\gamma_1, \ldots, \gamma_K)$$
$$\theta_k \sim p(\theta_k|\delta)$$

How to estimate when membership of y_i to components $1, \ldots, K$ is not known?

Finite Mixture Model: Estimation

Enter data augmentation! (Tanner Wong, 1987; *JASA*)
The idea:

- Introduce z_i = cluster membership for y_i and treat as missing data

$$
\begin{aligned}
p(y_i|\boldsymbol{\nu}) &= \sum_{k=1}^{K} p(y_i|z_i = k, \boldsymbol{\nu}) Pr(z_i = k|\boldsymbol{\nu}) \\
Pr(z_i = k|\boldsymbol{\nu}) &= \eta_k \\
p(y_i|z_i = k, \boldsymbol{\nu}) &= f(y_i|\theta_k)
\end{aligned}
$$

- Inference on z_i provides information on clustering

Finite Mixture Model: Estimation by MCMC

1. Sample $\boldsymbol{z}$ (Bayes' rule)

$$Pr(z_i = k|y_i, \boldsymbol{\nu}) = \frac{\eta_k f(y_i|\boldsymbol{\theta}_k)}{\sum_{j=1}^{K} \eta_j f(y_i|\boldsymbol{\theta}_j)}$$

$$z_i \sim MN(1, Pr(z_i = 1|y_i, \boldsymbol{\nu}), \ldots, Pr(z_i = K|y_i, \boldsymbol{\nu}))$$

2. Conditional on $\boldsymbol{z}$: Update $\eta_1, \ldots, \eta_K$

$$\eta_1, \ldots, \eta_K \sim \mathcal{D}(\delta_1 + n_1, \ldots, \delta_K + n_K)$$

3. Conditional on $\boldsymbol{z}$: Update $\theta_1, \ldots, \theta_K$

$$\theta_k \sim p(\boldsymbol{\theta}_k|\delta) \prod_{i:z_i=k} f(y_i|\boldsymbol{\theta}_k)$$

Finite Mixture Model: Estimation by MCMC

Available approaches in R:

- `R2OpenBUGS` (see `fmm_BUGS.R`)
- `bayesmix`

Or code from scratch:

- see `fmm_mvn.R` for Multivariate Normal example

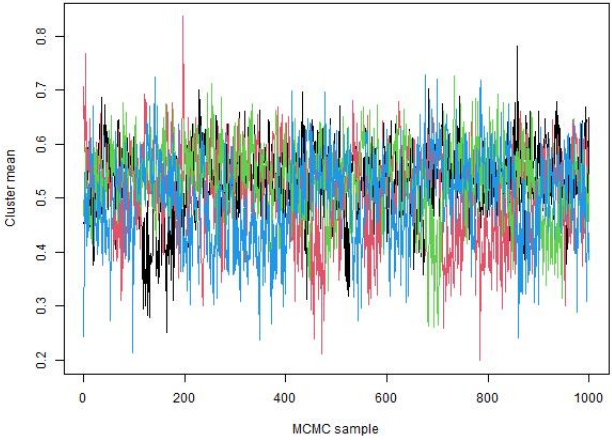
Label switching

Issue arises as likelihood is invariant to permutations of k e.g. $K = 3$

$$
\begin{aligned}
p(y_i|\boldsymbol{\nu}) &= \eta_1 p(y_i|\boldsymbol{\theta}_1) + \eta_2 p(y_i|\boldsymbol{\theta}_2) + \eta_3 p(y_i|\boldsymbol{\theta}_3) \\
&= \eta_3 p(y_i|\boldsymbol{\theta}_3) + \eta_2 p(y_i|\boldsymbol{\theta}_2) + \eta_1 p(y_i|\boldsymbol{\theta}_1) \\
&= \eta_2 p(y_i|\boldsymbol{\theta}_2) + \eta_3 p(y_i|\boldsymbol{\theta}_3) + \eta_1 p(y_i|\boldsymbol{\theta}_1)
\end{aligned}
$$

When sampling z_i, components can be relabelled $\rightarrow$ affects clustering inference

Label switching example



Label switching: Possible solutions

Prior constraints (not a good idea):

$$\eta_1 < \eta_2 < \ldots < \eta_K$$

Relabelling algorithms:

- Loss functions: minimise over all MCMC samples of z (Stephens, 2000)
- MAP estimate $\widehat{z}$ as 'pivot' (Marin et. al, 2005)

Label switching: Possible solutions

Similarity matrix, **S**:

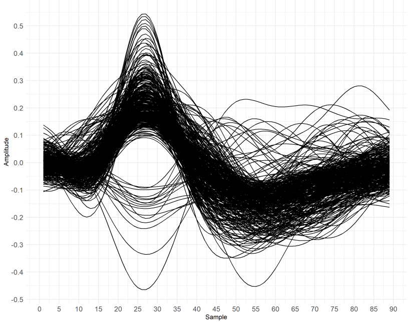
$$S_{ii'}^{(d)} = \begin{cases} 1 & \text{if } z_i^{(d)} = z_{i'}^{(d)} \\ 0 & \text{otherwise.} \end{cases}$$

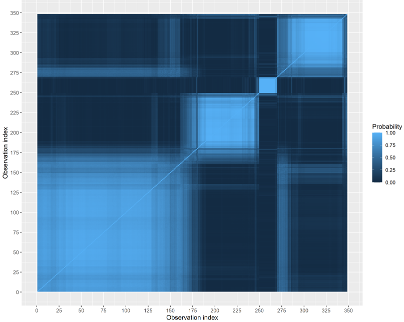
$$\overline{S} = \frac{1}{D} \sum_{d=1}^{D} S^{(d)}$$

R packages: `mcclust`, `label.switching`

Label switching

Example: Spike sorting, $K = 4$ clusters





Choosing K

Common information criteria:

- Akaike's Information Criterion (AIC)

$$AIC_K = -\log p(\mathrm{y}|\boldsymbol{\eta}^*, \boldsymbol{\theta}^*) + 2p_k$$

- Bayesian Information Criterion (BIC)

$$BIC_K = -\log p(\mathrm{y}|\boldsymbol{\eta}^*, \boldsymbol{\theta}^*) + p_k \log n$$

- Deviance Information Criterion (DIC)

$$DIC_K = -4E_{\boldsymbol{\eta},\boldsymbol{\theta}|\mathrm{y}}\left[\log p(\mathrm{y}|\boldsymbol{\eta}, \boldsymbol{\theta})\right] + 2\log f(\mathrm{y})$$

$$f(\mathrm{y}) = \prod_{i=1}^{n} \frac{1}{D} \sum_{d=1}^{D} \sum_{k=1}^{K} \eta_k^{(d)} f(y_i|\theta_k^{(d)})$$

1. Finite mixture models
2. Dirichlet Process Mixture models
3. Profile regression

Dirichlet Process mixture model: Motivation

General formulation:

$$p(y_i|\boldsymbol{\nu}) = \sum_{k=1}^{K} \eta_k f(y_i|\boldsymbol{\theta}_k)$$

In a finite mixture - assume K as fixed $\rightarrow$ model comparison problem

Alternative: Infer K as part of modelling

$$p(y_i|\boldsymbol{\nu}) = \sum_{k\geq 1} \eta_k f(y_i|\boldsymbol{\theta}_k)$$

Dirichlet Process mixture model: Setup

- Nonparametric approach to mixture modelling
- Does not estimate K directly; focus on clustering of individual parameters, θ_i

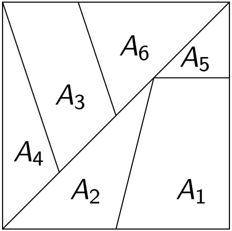
Dirichlet process (DP) prior:

$$\begin{aligned} G &\sim DP(\alpha, G_0) \\ G_0 &= E(G); \qquad \text{Base distribution} \\ \alpha &> 0; \qquad \text{Concentration parameter} \end{aligned}$$

Dirichlet Process mixture model: Setup

Each draw from a DP is itself a distribution:

$$G(A_1), \ldots, G(A_k)|\alpha, G_0 \sim D(\alpha G_0(A_1), \ldots, \alpha G_0(A_k))$$



"Discreteness property": multiple draws from $DP(\alpha, G_0)$ can take the same value; induces clustering behaviour

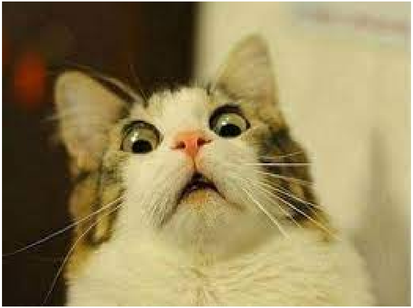
Dirichlet Process mixture model: Setup

DP as prior within mixture setting:

$$
\begin{aligned}
y_i|\boldsymbol{\theta}_i &\sim p(y_i|\boldsymbol{\theta}_i) \\
\boldsymbol{\theta}_i|G &\sim G \\
G &\sim DP(\alpha, G_0)
\end{aligned}
$$

- G is the mixing distribution
- G_0 prior distribution on unknown components
- α controls variation around G_0

Dirichlet Process mixture model: Estimation



How to sample from $DP(\alpha, G_0)$?!
What happened to η_k?!

- Stick breaking representation
- Pòlya Urn scheme/Chinese restaurant process

Stick breaking representation

G replaced by an infinite sum of weighted point masses:

$$\begin{aligned} G &\sim DP(\alpha, G_0) \\ G &= \sum_{k=1}^{\infty} \eta_k \delta_{\theta_k} \\ \theta_k &\sim G_0. \end{aligned} \tag{1}$$

$\eta_k; k = 1, \ldots$ are the "stick breaking weights".
Weights are drawn sequentially:

$$\begin{aligned} w_k|\alpha &\sim Beta(1, \alpha) \\ \eta_1 &= w_1 \\ \eta_k &= w_k \prod_{l=1}^{k-1} (1 - w_l). \end{aligned}$$

Stick breaking process

1

- Draw $w_1 \sim Beta(1, \alpha)$ and set $\eta_1 = w_1$

w_1	$1 - w_1$

- Draw $w_2 \sim Beta(1, \alpha)$ and compute $\eta_2 = w_2(1 - w_1)$

w_1	w_2	$(1 - w_2)(1 - w_1)$

- Draw $w_3 \sim Beta(1, \alpha)$ and compute $\eta_3 = w_3(1 - w_1)(1 - w_2)$

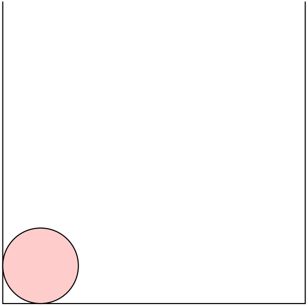
w_1	w_2	w_3	$(1 - w_3)(1 - w_2)(1 - w_1)$

As $K \to \infty$

$$p(y_i|\boldsymbol{\nu}) = \sum_{k=1}^{K} \eta_k p(y_i|\boldsymbol{\theta}_k)$$

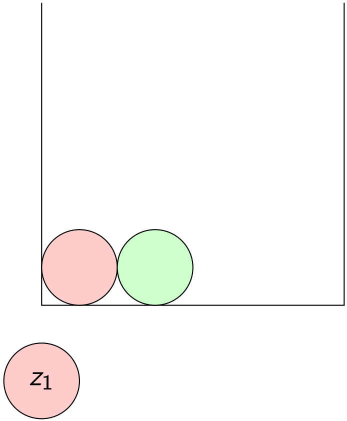
The Pòlya Urn scheme

Good analogy for implied clustering behaviour
Begin with α red balls in an urn:



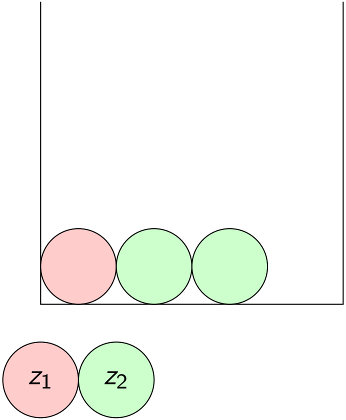
The Pòlya Urn scheme

If a red ball is drawn, record colour and replace with a ball of a new colour:

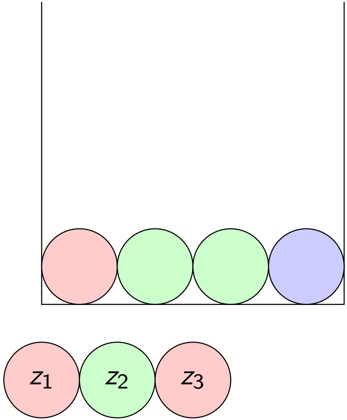


The Pòlya Urn scheme

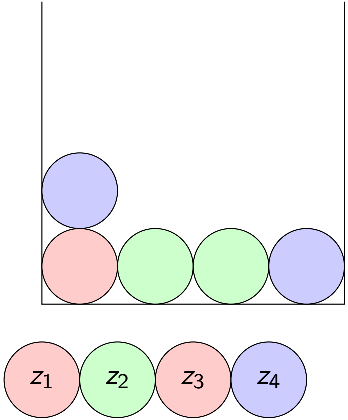
If a non-red ball is drawn, record colour and replace with a ball of the same colour:



The Pòlya Urn scheme



The Pòlya Urn scheme



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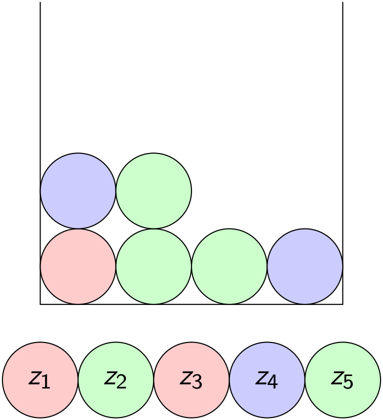

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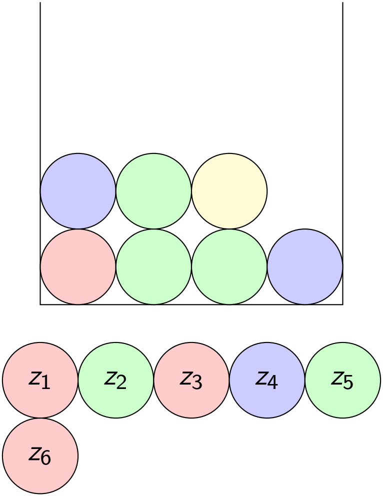

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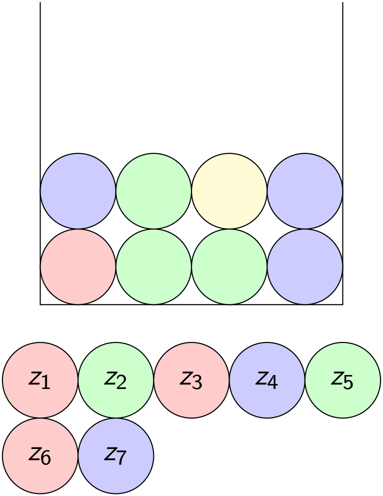

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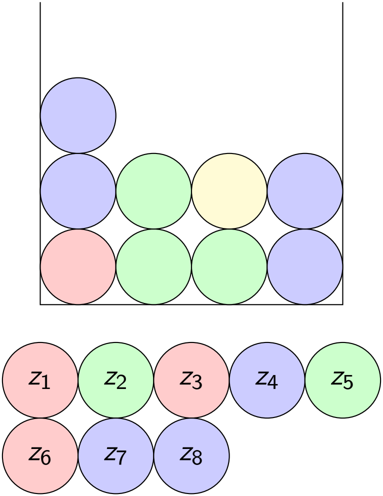

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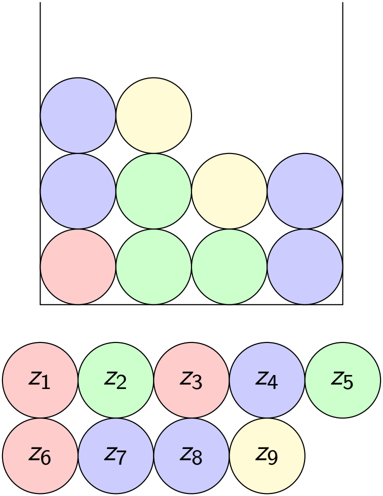
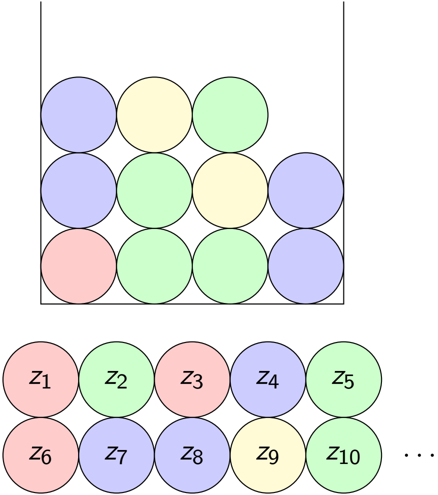


The Pòlya Urn scheme



- The more often a colour is drawn, the more likely it is to

Dirichlet Process mixture model: Estimation

R packages

- `dirichletprocess`
- https://rdrr.io/cran/NPflow/man/DPMGibbsN$_SeqPrior.html$`PReMiuM`

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