# Finding structures in observations: consistent(?) clustering analysis.

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**OBayes** Conference

(Santa Cruz)

10 September 2022

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## Clustering:

- "unsupervised learning"
- requires data, but no labels
- detect patterns, e.g.
  - online search results
  - customer shoppint patterns
  - effect of pollution
  - animal behaviours
  - cells, tissues, etc
  - regions of images
- common initial analysis: useful when you have no idea
- how to interpret results?



## Clustering algorithms

### Partitioning algorithms:

- k-means
- mixture models
- spectral custering



### Hierarchical algorithms:

- bottom-up, agglomerative
- top-down, divisive



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## Examples of clustering

### Clustering gene expression data:

### Find clusters of cells with similar biological expression



### An iterative algorithm:

- **Initialise:** pich *K* random points as cluster centers
- Alternate:
  - assign data points to closest cluster center
  - change the cluster center to the average of its assigned points
- **Stop:** when there is no change in assignments



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### K-means



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Consider the following mixture model

$$g(y; \psi) = \sum_{j=1}^{K} p_j f_j(y; \theta_j)$$

where

• 
$$\psi = (\theta_1, \cdots, \theta_K, p_1, \cdots, p_K)$$

• 
$$p_j \ge 0$$
 for  $j = 1, \cdots, K$ 

• 
$$\sum_j p_j = 1$$

•  $f_j(\cdot)$  is any probability distribution

These models provide a flexible tool for statistical inference (even in a nonparametric setting, see Lindsay (1995), Roeder (1992) and Roeder and Wasserman (1997)).



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Often in Bayesian inference, we want to reduce the effect of the prior on the posterior distribution, in case we do not have strong prior information.

Sometimes so-called "improper" priors are used

$$\int_{\Theta} \pi( heta) d heta = \infty.$$

This is not a pdf (or a pmf), therefore the Bayes' theorem cannot be applied.

However they are used in practice as limit of proper prior distributions, when the assure a proper posterior distribution.

It is delicate to produce a noninformative prior for the parameters of a mixture model, since they are often *improper*.

## Why can't we use improper priors? Example:

Consider independent improper priors

$$\pi(\theta_1,\cdots,\theta_K) \propto \prod_{j=1}^K \pi(\theta_j)$$

such that  $\int_{\Theta} \pi(\theta_j) d\theta_j = \infty$ 

The mixture model is a classical example of latent variable model, then it can be rewritten as

$$g(y; \psi) = \sum_{S = \mathscr{S}_k} \prod_{j=1}^{K} f(y; S, \theta_j) \pi(\theta_j) \pi(S \mid p) \pi(p)$$

where the summation runs over all  $k^N$  possible classifications *S*. Then the complete-data likelihood is non-informative if there is an empty component (let's say the *j*-th)

$$\int \prod_{i:S_i=j} f(y_i;\theta_j) \pi(\theta_j) d\theta_j \propto \int \pi(\theta_j) d\theta_j = \infty$$

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### Random partition models

• A random partition model is a probability distribution over  $\mathscr{P}_n$ 

$$\{p(\rho_n = (S_1, \ldots, S_K)) : \rho_n \in \mathscr{P}_n\}$$

• One main approach is to to define  $p(\rho_n)$  through discrete random probability measures

$$f(y_1, \dots, y_n | \theta_1, \dots, \theta_n) = \prod_{i=1}^n f(y_i | \theta_i)$$
$$\theta_1, \dots, \theta_n | G \stackrel{i.i.d.}{\sim} G$$
$$G \sim \text{discrete RPM}$$

For example, if  $G(\cdot) = \sum_{h=1}^{K} p_h \delta_{\psi_h}$  with  $P(\sum_{h=1}^{K} p_h = 1) = 1$ , then

$$g(y_i|\{\psi_h\}) = \sum_{h=1}^{K} p_h f(y_i|\psi_h)$$

- Discreteness of G implies existence of ties among  $\theta_1, \ldots, \theta_n$
- If ψ<sub>1</sub>,..., ψ<sub>K</sub> denote the corresponding unique values then we can define ρ<sub>n</sub> through indicators given as

$$c_i = j \Leftrightarrow \theta_i = \psi_j$$
 or equivalently  $\theta_i = \psi_{c_i}$ 

and so  $S_j = \{i \in [n] : \theta_i = \psi_j\}$ , where  $[n] = \{1, ..., n\}$  is the set of n indices.

• This is an induced random partition model.

- ρ<sub>n</sub> = (S<sub>1</sub>,...,S<sub>K</sub>) a partition of [n] into K = |ρ<sub>n</sub>| ≥ 1 nonempty (and mutually exclusive) subsets;
- 𝒫<sub>n</sub>: set of all partitions of [n];
- the size of  $\mathscr{P}_n$  increases as the Bell number; e.g.  $B_{10} = 115,975$

### Finite mixture models

• Consider  $K \sim p_K(k)$ 

$$y_i|K = k, p_1, \dots, p_K, \theta_1, \dots, \theta_K \stackrel{i.i.d.}{\sim} \sum_{h=1}^K p_h f(y_i|\theta_h)$$
$$\theta_1, \dots, \theta_k|K = k \stackrel{i.i.d.}{\sim} p_0(\theta)$$
$$(p_1, \dots, p_k)|K = k \sim Dir(\gamma, \dots, \gamma)$$

The induced partition model is then

$$p(\rho_n = (S_1, \ldots, S_K)) = \left(\sum_{h=1}^{\infty} \frac{h_{(k)}}{(\gamma h)^{(n)}} p_K(h)\right) \left(\prod_{s \in (S_1, \ldots, S_K)} \gamma^{|s|}\right)$$

where  $x^{(m)} = x(x+1)...(x+m-1)$  and  $x_{(m)} = x(x-1)...(x-m+1)$ .

- One approach consists in fixing K to a large value and use inference to estimate some of the weights as equal to zero, in order to identify the correct k < K number of clusters.</li>
- Playing on the prior for  $(p_1, \ldots, p_K)$
- [Rousseau and Mengersen (2011)] show the asymptotic behaviour of the posterior distribution in a mixture model for overfitted mixtures: the posterior distribution concentrates on a sparse representation of the true density; this is exhibited by a subset of components that adequately describe the density remaining and any superfluous components becoming empty.
- IMPORTANT: need for a prior on the weights that favour small weights (Dirichlet with parameters 1/2).

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We recall that the Jeffreys prior was introduced by Jeffreys (1939) as a default prior based on the Fisher information matrix

$$\pi^{\mathsf{J}}(\theta, \mathbf{p}) \propto |I(\theta, \mathbf{p})|^{1/2} = \det\left(\mathbb{E}_{g}\left[-rac{d^{2}}{d\psi^{2}}\log g(y; \mathbf{p}, \theta)
ight]
ight)^{1/2}$$

- when using the Jeffreys' prior for all the parameters of the model, the posterior is improper (OH NO!)
- but when the Jeffreys' prior is used only for the weights, it can be shown that it leads to the same results as Rousseau & Mengersen (2011)!

### Jeffreys prior for the weights

Instead, we fix the Jeffreys prior only for the weights conditionally on the other parameters

 $\pi^{J}(p_1,\ldots,p_K|\theta_1,\ldots,\theta_K) \propto |I(p_1,\ldots,p_K)|^{1/2}$ 



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The induced partition model is then

$$p(\rho_n = (S_1, \dots, S_K)) = \left(\sum_{h=1}^{\infty} \frac{h_{(k)}}{(\gamma h)^{(n)}} p_K(h)\right) \left(\prod_{s \in (S_1, \dots, S_K)} \gamma^{|s|}\right)$$

where  $x^{(m)} = x(x+1)...(x+m-1)$  and  $x_{(m)} = x(x-1)...(x-m+1)$ .

For model

$$g(y; \psi) = \sum_{j=1}^{K} p_j f_j(y; \theta_j)$$

the prior can be specified as

$$\pi(k,\mathbf{p},\theta) = p_{\mathcal{K}}(k)\pi(\mathbf{p} \mid k)\pi(\theta \mid k).$$

The posterior for k is then given by

$$p_{\mathcal{K}}(k \mid y) \propto \int f(y \mid k, \mathbf{p}, \theta) \times p_{\mathcal{K}}(k) \pi(\mathbf{p} \mid k) \pi(\theta \mid k) d\mathbf{p} d\theta.$$

- Although for practical purposes the range of values K can take is finite, it may be appropriate to define a prior over N.
- In fact, by truncating the support of *K* there may be possible distortions of the posterior around the boundary, affecting the inferential results.
- **BUT** the prior on *K* must be proper, as proved by Nobile (2005).
- Remember the **inconsistency problems** in the nonparametric setting see Miller and Harrison (2014).

- $K \sim Unif(0, 30)$  (Richardson and Green, 1997)
- $K \sim Pois(1)$  (Nobile and Fearnside, 2007)
- K ~ BNB(1, a, b) (Grazian et al. 2020, Früwirth-Schnatter et al., 2021)
  - Früwirth-Schnatter et al. (2021) propose to combine a prior on K with an adaptive prior on the weights  $(p_1, \ldots, p_K) \sim Dir(\frac{\alpha}{K}, \ldots, \frac{\alpha}{K})$  "dynamic" version of the mixtures



Früwirth-Schnatter et al., 2021

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**Idea:** inconsistency problems can be prevented by penalising larger values  $\rightarrow$  we can define the prior on K with a loss-based approach.

To obtain the **loss-based prior** on K, we define the prior on K by assigning a prior on the space of models determined by the mixtures with k = 1, 2, ... components.

- we can assign a *worth* to each mixture
- we include a component of loss due to the complexity of the model

$$Loss(k) = Loss_I(k) + Loss_C(k)$$

## A loss-based prior: information loss [Grazian et al., 2020]

The quantification of the loss comes from Berk (1966): *if the model is misspecified, the posterior distribution asymptotically tends to accumulate at the most similar model so to minimise the loss in information, in terms of Kullback-Leibler divergence* 

If we consider a mixture  $M_s = \{g_s(x|\psi_s), \pi_s(\psi_s)\}$  (where  $\psi_s = (p_s, \theta_s)$ 

$$\operatorname{Loss}_{I}(k) = \mathbb{E}_{\pi_{s}}\left\{ \inf_{\psi_{m}, m \neq j} D_{\mathcal{K}L} \left( g_{s}(x|\psi_{s}) \| g_{m}(x|\psi_{m}) \right) \right\},$$

The above loss is linked to the prior mass by means of the *self-information* loss function which associate a loss to a probability statement. As such,

$$p_{\mathcal{K}}(k) \propto \exp\left\{\operatorname{Loss}_{I}(k)\right\}.$$

The loss attains its minimum at zero: Consider mixture  $g_k = \sum_{j=1}^k p_j f_j(x|\theta_j)$  and  $g_{k+1} = \sum_{j=1}^k \breve{p}_j f_j(x|\breve{\theta}_j) + \breve{p}_{k+1} f_{k+1}(x|\breve{\theta}_{k+1})$ ; the minimum is obtained when  $\breve{p}_j = p_j$  and  $\breve{\theta}_j = \theta_j$  and  $\breve{p}_{k+1} = 0$ .

To fully describe the *worth* of a mixture model it is also necessary to take into consideration its complexity.

If we keep the mixture model with k components, the loss would be related to the number of parameters that have to be estimated, and therefore the number of components.

$$Loss_C(k) = U(keep \ k) = -c \cdot k.$$

Therefore,

$$p_{\mathcal{K}}(k) \propto \exp\{-c \cdot k\},\$$

where c > 0 is included as loss functions are defined up to a constant.

### Theorem

Consider the prior distribution for the number of components of a finite mixture model, where we set  $p = \exp\{-c\}$  and k = 1, 2, ... If we choose  $p \sim \text{Beta}(\alpha, \beta)$ , with  $\alpha, \beta > 0$ , then

$$p_{\mathcal{K}}(k|p)=p^{k-1}(1-p),$$

which is a geometric distribution with parameter 1 - p, and

$$p_{\mathcal{K}}(k) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{\Gamma(k+\beta-1)\Gamma(\alpha+1)}{\Gamma(k+\alpha+\beta)},$$

which is a beta-negative-binomial distribution where the number of failures before the experiment is stopped is equal to 1, and shape parameters  $\alpha$  and  $\beta$ .

The linear complexity loss is a choices; other choices are also possible.

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### The prior $p_{\mathcal{K}}(k)$ just defined

- is defined on the whole support of K,  $\mathbb N$
- is proper
- has moments

$$\mathbb{E}(\mathcal{K}) = \mathbb{E}(\mathbb{E}\{\mathcal{K}|p\}) = \mathbb{E}(p^{-1}) = \frac{\alpha + \beta - 1}{\alpha - 1}, \quad \text{for } \alpha > 1,$$
$$\operatorname{Var}(\mathcal{K}) = \mathbb{E}(\operatorname{Var}\{\mathcal{K}|p\}) + \operatorname{Var}(\mathbb{E}\{\mathcal{K}|p\}) = \frac{\alpha\beta(\alpha + \beta - 1)}{(\alpha - 2)(\alpha - 1)^2}, \quad \text{for } \alpha > 2.$$

where  $\beta$  can be used to control how many components we assume a priori and  $\alpha$  can be used to control the variance.

## The galaxy dataset



Galaxy Dataset

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Image: A matrix

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Suppose that the observations depend on a covariate, e.g. they are time-dependent.  $\rightarrow$  we can use hidden Markov models! Let

- $\{t_1, t_2, \dots, t_T\} \equiv \mathscr{T}$ : set of observed time points
- $\mathbf{y} = {\{\mathbf{y}_t\}_{t \in \mathscr{T}}}$ : the data
- c = {c<sub>t</sub>}<sub>t∈𝔅</sub>: a latent variable indicating the cluster each observation belongs to, with c<sub>t</sub> ∈ {1,2,...,K} ≡ 𝔅 and K

We assume that the data come from a mixture-type model

$$g(\mathbf{y}|\mathbf{c},\{\boldsymbol{\theta}_k\}_{k\in\mathscr{K}}) = \prod_{t\in\mathscr{T}}\prod_{k\in\mathscr{K}}f(y_t|\boldsymbol{\theta}_k)^{\mathbb{I}_k(c_t)}$$

i.e. given the latent variables  $\mathbf{c}$ , the observations  $y_t$  are independent.

One possible solution

$$g(\mathbf{y}|\mathbf{c}, \{\theta_k\}_{k \in \mathscr{K}}) = \prod_{t \in \mathscr{T}} \prod_{k \in \mathscr{K}} f(y_t|\theta_k)^{\mathbb{I}_k(c_t)},$$
$$c_t \sim \mathsf{Discrete}(\mathbf{p}_t),$$
$$\mathbf{p}(t) \sim \mathsf{LogitGP}(\mathbf{A}, \mu(t), \mathbf{C}(h))$$

So that the probabilities  $\mathbf{p}_t = {\{\mathbf{p}_{t,k}\}}_{k \in \mathcal{K}}$  are discrete-time observations of an underlying and non-observed continuous-time process  $\mathbf{p}(t)$ .

We have that

- A is a co-regionalization matrix
- $\mu(t)$  is a mean function
- C(h) is a correlation function with h being a temporal distance

[Aitchison, 1986] proposed the LogitN distribution to model compositional data as an alternative to the Dirichlet distribution.

The vector  $\mathbf{p}_t$  is defined as

$$p_{t,k} = rac{e^{\omega_{t,k}}}{\sum_{j=1}^{K} e^{\omega_{t,j}}}, \quad k \in 1, \dots, K$$

where  $\omega_{t,k}$  are real valued variables.

**Remark:** adding a constant to each  $\omega_{t,k}$  produces the same vector of probabilities, and an identifiability constraint is therefore needed; the K-th element is set to zero ( $\omega_{t,K} = 0$ ) treated as the *reference element*.

 $\omega_t$  can be the realisation of a K-1 dimensional GP  $\omega(t)$ .

Attention must be paid! The covariance among each element and the sum of all the element is

$$\operatorname{Cov}(p_{t,k}, p_{t,1} + \dots + p_{t,k} + \dots + p_{t,K}) = 0$$

where  $p_{t,1} + \cdots + p_{t,k} + \cdots + p_{t,K} = 1$ . Therefore we have

$$-\mathsf{Var}(p_{t,k}) = \sum_{\substack{h=1\\k\neq h}}^{K} \mathsf{Cov}(p_{t,k}, p_{t,h}).$$

Aitchison (1986) pointed out that a more consistent measure of dependence between compositional elements can be measure as

$$\tau_{ij,kl}(t,t') = \mathsf{Cov}\left(\log\frac{p_{t,i}}{p_{t,k}},\log\frac{p_{t',j}}{p_{t',l}}\right), i,j,k,l \in 1, \dots, K,$$

## The covariance of the $\mathbf{p}_t$

Let's keep things simple and suppose that  $\mathbf{p}_t \sim LogitN(\mu_t, \mathbf{\Sigma}_t)$ , where  $\mu_t$  is K-1 dimensional vector and  $\mathbf{\Sigma}_t$  is a  $(K-1) \times (K-1)$  square matrix.

• It can be proved that a *LogitN* process has independent components (in term of log-ratio), i.e.  $\tau_{ij,kl}(t,t') = 0$  for arbitrary *i*, *j*, *k* and *l*, at time lag |t - t'| only if the variance of the Gaussian variable is

$$\boldsymbol{\Sigma}_{t,t'} = \begin{pmatrix} a_1(t,t') + a_K(t,t') & a_K(t,t') & \dots & a_K(t,t') \\ a_K(t,t') & a_2(t,t') + a_K(t,t') & \dots & a_K(t,t') \\ \dots & \dots & \dots & \dots \\ a_K(t,t') & a_K(t,t') & \dots & a_{K-1}(t,t') + a_K(t,t') \end{pmatrix}$$

where the element  $[\mathbf{\Sigma}_{t,t'}]_{i,j}$  is  $\tau_{ij,KK}(t,t')$ .

• The elements of  ${\bf p}$  are iid if  ${\boldsymbol \mu}_t = {\bf 0}$  and

We introduce an auxiliary K-dimensional GP  $\gamma(t)$ , From  $\gamma(t)$ , we construct  $\omega(t)$  as

$$egin{aligned} &\omega_k(t) = \gamma_k(t) - \gamma_{\mathcal{K}}(t), \ &\gamma(t) = \mu(t) + \mathbf{A}\gamma^*(t), \ &\gamma^*_k(t) \sim \mathsf{GP}(0, C_k(h)). \end{aligned}$$

where

- A is a coregionalization matrix, which we require to be non-negative definite and symmetric
- $\mu(t)$  is a mean function
- C(h) is a vector of correlation functions

Matrix **A** introduces dependence between the elements of  $\gamma(t)$ , and

 $\pmb{\Sigma} = \pmb{A}\pmb{A}'$ 

is the covariance of  $\gamma(t)$ .

The explicit relation between  $\boldsymbol{\mathsf{A}}$  and  $\boldsymbol{\Sigma}$  is

$$\mathbf{A} = \mathbf{\Delta} \mathbf{\Xi}^{\frac{1}{2}} \mathbf{\Delta}',$$

where

- $\Delta$  is the matrix of the eigenvectors of  $\Sigma$
- $\Xi$  is the diagonal matrix of the eigenvalues of  $\Sigma$

Then

$$\mathbf{p}(t) \sim \mathsf{LogitGP}(\mathbf{A}, \mu(t), \boldsymbol{C}(h))$$

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It is important to highlight that  $\gamma(t)$  is **not identifiable** and any inference about  $\mathbf{p}_t$  is in fact made by looking at  $\omega_t$  through equation.

$$p_{t,k} = \frac{e^{\gamma_{t,k}-\gamma_{t,K}}}{\sum_{j=1}^{K} e^{\gamma_{t,j}-\gamma_{t,K}}} = \frac{e^{\gamma_{t,k}}}{\sum_{j=1}^{K} e^{\gamma_{t,j}}}, \quad k \in 1, \dots, K.$$

With respect to the case where  $\omega_{t,K}$  must be set to zero, this equation has a more symmetric form, since all the components of  $\mathbf{p}_t$  are written in terms of exponentials of  $\gamma_k(t)$  and there is no reference element.

It can be proved that this model assures

- invariance from the choice of the reference element;
- invariance with respect to the reordering of the labels;
- the expected structure of the covariance matrix among times, when defined on  $\tau_{ij,kl}(t,t')$  elements.

A mixture model can be extended to consider infinite components:

$$y_i | heta_i \sim f(y_i | heta_i)$$
  $i = 1, ..., n$   
 $heta_i | heta \sim G$   
 $G | lpha, G_0 \sim DP(lpha, G_0),$ 

and, since G is almost surely discrete, this model can be rewritten as

$$y_i \sim \sum_{h=1}^{\infty} \pi_h f(y_i | \psi_h) \qquad i = 1, \dots, n$$

where  $\psi_1, \psi_2, \ldots$  are independent draws from the base distribution  $G_0$ .

The EPPF of the DP is explicitly available; if  $G \sim DP(\alpha, G_0)$ , then

$$p(\rho_n = (S_1, \ldots, S_K)) = \frac{\alpha^K \prod_{h=1}^K (n_h - 1)!}{\prod_{i=1}^n (\alpha + i - 1)!}.$$

which is known as Ewens distribution.

(Generalization to other processes, like the PY process are available) And the conditional EPPF for a DP mixture model, induced for a given number of clusters K = k, is

$$p_{DP}(\rho_n = (S_1, ..., S_k) | \mathcal{K} = k) = \frac{1}{Const} \prod_{h=1}^k \frac{1}{n_h}$$

However, it can be shown that this EPPF favours unbalanced partitions with some small values of  $n_h$  (look at the inverse dependence on  $n_h$ )  $\rightarrow$  this model is inconsistent for clustering!

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## CASE 4b: Adding covariates - Grazian (2022+)

Suppose  $Y_t(s)$  come be represented as an infinite mixture model:

$$g(y_t(s)|\pi, heta) = \sum_{k=1}^{\infty} \pi_{t,k}(s)g(y_t(s)| heta_k)$$

where the mixing probability  $\pi_{t,k}(s)$  is the probability that the location s belongs to component k at time t.

The mixing weights are built similarly to the spatial stick-breaking:

$$\begin{aligned} F_t(s) &= \sum_{k=1}^{\infty} \pi_{t,k}(s) \delta_{\theta_k} \quad s \in \mathscr{D}, t > 0 \quad \text{where} \\ \pi_{t,1}(s) &= V_{t,1}(s), \quad \pi_{t,k}(s) = V_{t,k}(s) \prod_{j=1}^{k-1} (1 - V_{t,j}(s)) \quad \text{for } k = 2, \dots \\ V_{t,k}(s) &= w_k(s, \psi, t, \zeta) V_k \\ V_k &\sim Beta(a, b) \\ \theta_k &\sim F_0. \end{aligned}$$

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Consistently estimating the number of clusters in a Bayesian way is difficult.

### However

- consistency can be found for overfitted mixtures
- the prior may have an important role
- advantage of reducing the number of necessary assumptions and inputs
- easy extension to multivariate setting

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