

A log-ratio approach to cluster analysis of count data when the total is irrelevant

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Compositional data analysis

- **Compositional data** (CoDa), (p_1, \dots, p_D) , are quantitative descriptions of the parts of some whole, conveying **relative information**. CoDa are commonly expressed in proportions, percentages, or ppm (Aitchison, 1986).
- The simplex

$$S^D = \left\{ (p_1, \dots, p_D) \mid p_i > 0, \sum_{i=1}^D p_i = \kappa \right\},$$

is the sample space of CoDa.

- **Log-ratios** of parts handle relative information and satisfy desirable properties such as scale invariance and subcompositional coherence:

$$\log \left(\frac{p_i}{p_j} \right), \log \left(\frac{p_j}{\sqrt[D]{\prod_{\ell=1}^D p_\ell}} \right), \sqrt{\frac{j}{j+1}} \log \frac{\sqrt[j]{\prod_{\ell=1}^j p_\ell}}{p_{j+1}}, \dots$$

CoDa and the zero problem

- Zeros prevent from using log-ratios. Most proposals have been focused on the continuous case (**zCompositions** R package; Palarea-Albaladejo & Martín-Fernández, 2015).
- **Compositional count data sets:** discrete vectors of number of outcomes falling into mutually exclusive categories.

Municipality	jxsi	psc	pp	catsp	cs	cup
S. Jaume de F.	14	1	0	2	0	5
Gisclareny	20	0	0	0	1	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮
L'Hosp. de Llob.	23843	28947	14336	16855	29773	7528
Barcelona	326376	100806	80529	85841	155361	87774

- **Assumption 1:** The relative information is relevant, the total is not.
- **Assumption 2:** The probability of a part different of zero is not zero. Count zeros due to sampling limitations.

Parametric approaches to cluster compositional count data set (1)

Two sources of variability are considered:

Count (observations) Compositional (probabilities)

- **Compositional** and **count** variability not taken into account. Classical methods applied to observed counts (p.e. Gaussian mixtures with the counts).
- **Count** variability taken into account, but not **compositional** variability. Mixtures of multinomial distributions.
- **Compositional** variability taken into account, but not **count** variability. Zero multiplicative replacement methods.
 - Dirichlet prior (Martín-Fernández *et al.*, 2015)
 - Log-ratio normal prior (Comas-Cufí *et al.*, 2019)

Parametric approaches to cluster compositional count data set (2)

- **Compositional** and **count** variability taken into account.
 - *Topic models.* Mixture of multinomials where mixing proportions are modelled in the Simplex.
 - Latent Dirichlet Allocations (Blei *et al.* 2003)
 - Correlated Topic Models (Blei & Lafferty, 2007)
 - *Mixtures of compounding distributions.*
 - Mixtures of Dirichlet-multinomial distributions (Holmes *et al.*, 2012)
 - Mixtures of log-ratio-normal-multinomial distributions (Comas-Cufí *et al.*, 2017)

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Main limitations

- Dirichlet-based approaches have **modelling difficulties**.
- Gaussian-based approaches have **estimation difficulties**.

Our proposal

Classical clustering approaches applied to cluster count data

1. Dealing with zeros.

- Dirichlet-multinomial (DM) distribution: conservative in keeping the covariance structure observed in the original count data set. The regression toward the mean is moderate.
- Zero replacement: conservative in keeping covariance structure observed in the count data set. Counts with small parts tend to define clusters by themselves.

2. **Compositional variability.** Model your data using a generic distribution defined on the Simplex. Gaussian mixtures are easy to estimate.
3. **Count variability.** Create B new samples using the posterior distribution, and find clusters using classical methods on its log-ratio coordinates.
4. **Consensus clustering.** Use a clustering ensemble method to build a final cluster (e.g. majority voting (Dudoit & Fridlyand, 2003)).

Example: 2017 Catalan regional election

Multivariate count data set

- 947 municipalities. To illustrate the approach we only consider three parts obtained with the following amalgamations.
 - Pro-independence parties (ind):** CUP (cup), Esquerra Republicana de Catalunya (erc), Junts per Catalunya (jxcat).
 - Anti-independence parties (esp):** Ciutadans (cs), Partit Popular (pp), Partit Socialista de Catalunya (psc).
 - Mixed opinions (other):** Catalunya si que es pot (catsp), others (other).

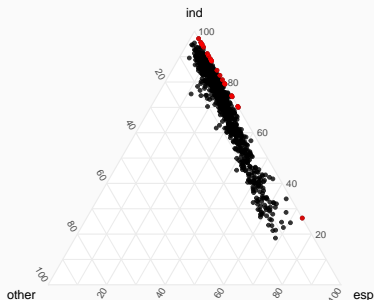
mun	catsp	cs	cup	erc	jxcat	other	pp	psc
Abella de la Conca	4	9	8	30	50	0	0	13
Abrera	815	2559	198	1411	634	158	321	1487
Agramunt	80	472	100	1148	956	7	125	161
Aguilar de Segarra	1	12	38	37	85	0	3	9
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

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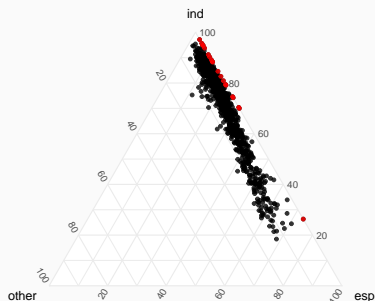
mun	ind	esp	other
Abella de la Conca	88	22	4
Abrera	2243	4367	973
Agramunt	2204	758	87
Aguilar de Segarra	160	24	1
⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮

Dealing with zeros



- Most municipalities lie between **ind** and **esp** parties.
- Some municipalities have some count zero (●).

Dealing with zeros



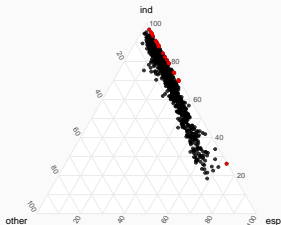
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 - Some municipalities have some count zero (●).
- **We will deal with zeros first.**

Dealing with zeros

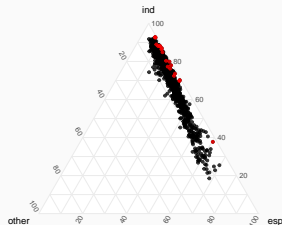
Here, we consider two different approaches:

- Geometric Bayesian multiplicative (Martín-Fernández, 2015), and
- Dirichlet-multinomial smoothing after replacing by the expected posterior probabilities.

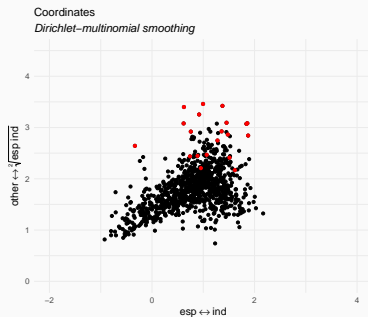
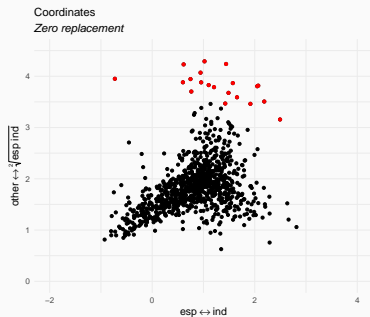
Zero replacement



Dirichlet-multinomial smoothing

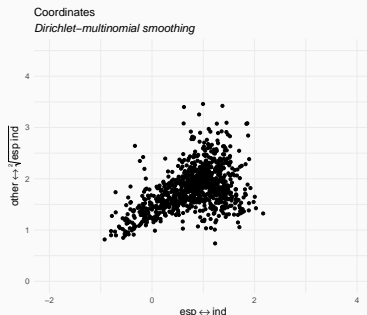
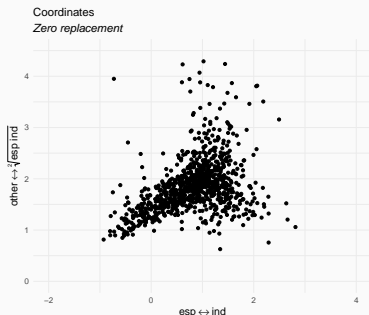


Dealing with zeros



Basis \mathcal{B}	ind	esp	other
B1	1	-1	0
B2	1	1	-1

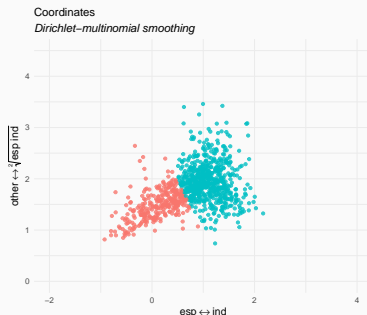
Clustering directly in count data



We can cluster our compositional data for example using k -means.

- Duda-Hart test was used to discard one cluster.
- Calinski-Harabasz index was used to select k between 2 and 10.

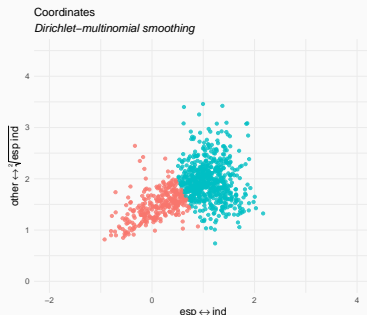
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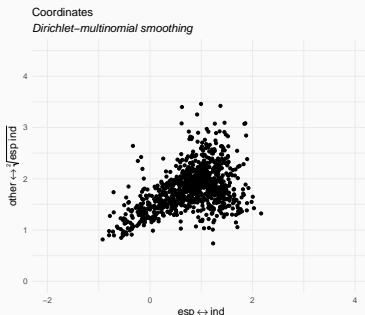
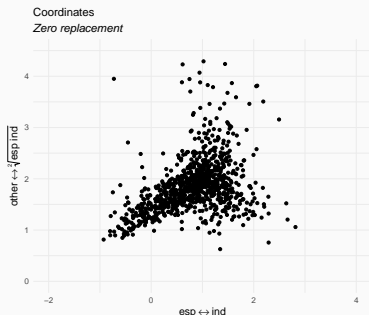
Clustering directly in count data



Limitations

- In the zero-replacement approach, observations with a small amount of counts tend to create clusters.
- In DM smoothing results can be affected by the Dirichlet prior.

Compositional variability

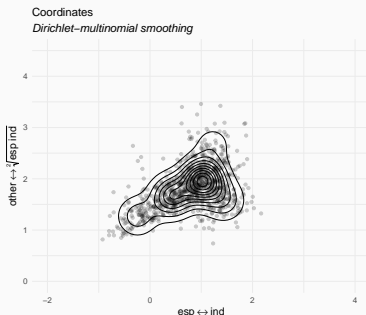
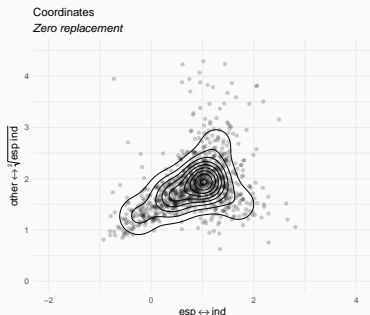


Modelling using Gaussian mixtures

Find a distribution to model the original sample. Mixtures of Gaussian distribution are a good option (Nguyen & McLachlan, 2018).

→ According to BIC criterion, a mixture of 7 and 5 spherical Gaussian distributions with equal volume were respectively used.

Compositional variability

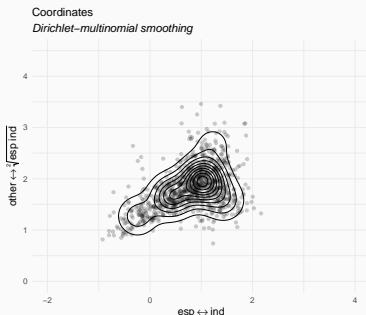
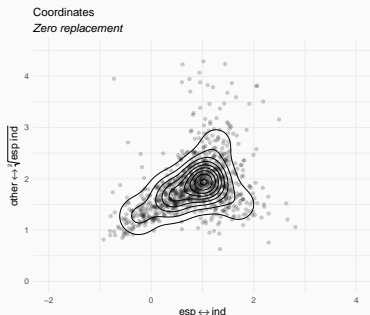


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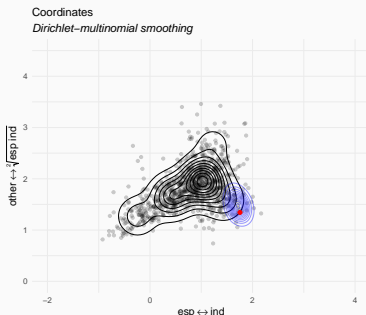
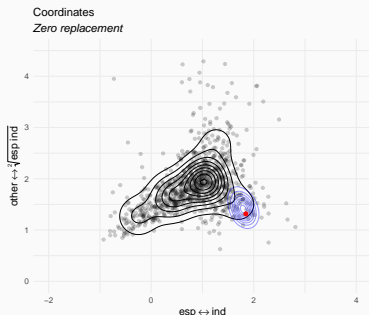


Sampling from the posterior distribution

For each count observation \mathbf{x}_i , we sample from the posterior distribution $P(\mathbf{h} \mid \mathbf{x}_i; f)$, where f is the mixture of Gaussian distributions.

- Metropolis–Hastings using $g(\mathbf{h}) = f(\mathbf{h}) \cdot \text{Mult}(\mathbf{x}_i; \text{ilr}_B^{-1}(\mathbf{h}))$ with proposal step defined by the Laplace approximation of $P(\mathbf{h} \mid \mathbf{x}_i; f)$ centred at zero.

Count variability

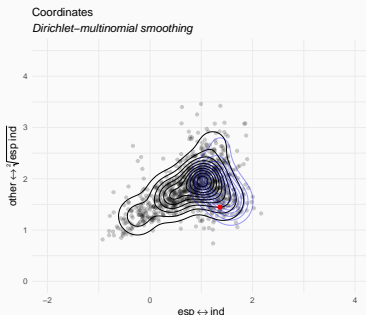
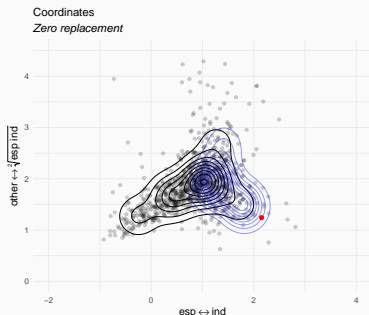


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- $i = \text{"Argelaguer"} , \mathbf{x}_i = (\text{ind: } 259, \text{esp: } 19, \text{other: } 14)$

Count variability

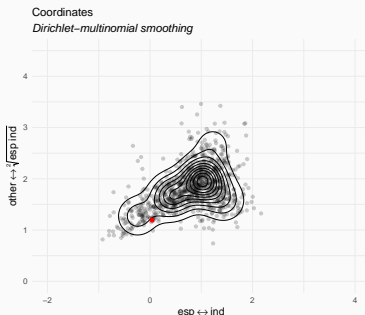
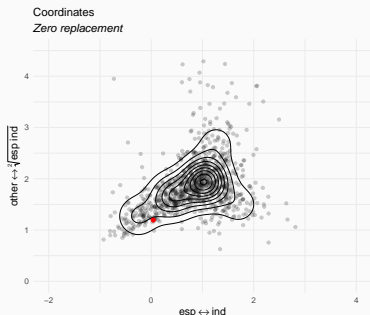


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- $i = \text{“Gisclareny”}$, $\mathbf{x}_i = (\text{ind: } 1, \text{esp: } 21, \text{other: } 1)$

Count variability

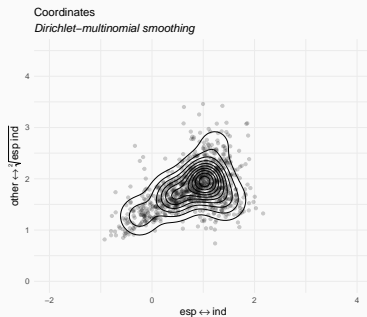
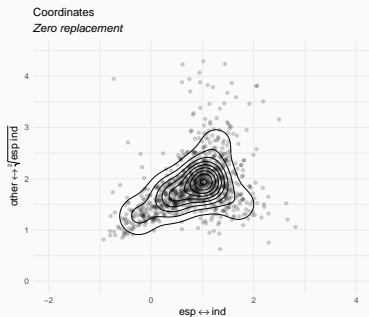


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- $i = \text{"Barcelona"}$, $\mathbf{x}_i = (\text{ind: } 429\,782, \text{esp: } 405\,924, \text{other: } 96\,748)$

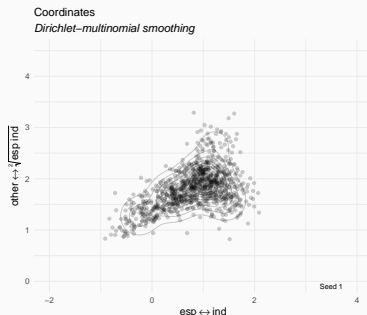
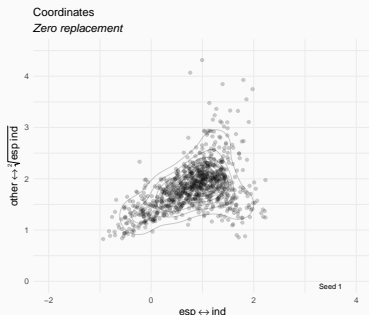
Compositional and count variability



Creating new samples

→ Using the posterior distribution we can create B new samples ($B = 100$),

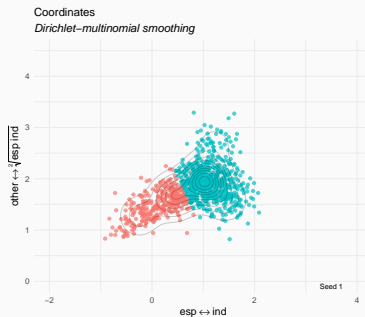
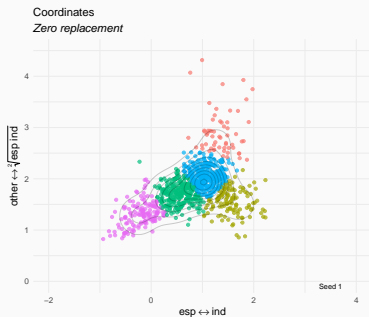
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Creating new samples

- Using the posterior distribution we can create B new samples ($B = 100$),
- and applying a clustering algorithm (k -means, $k \in \{2, \dots, 10\}$, Calinski-Harabasz index).

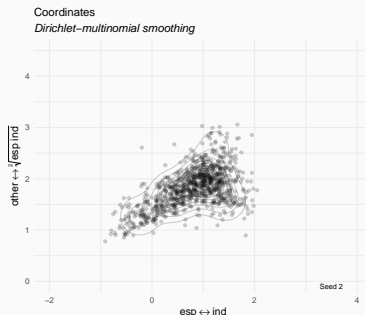
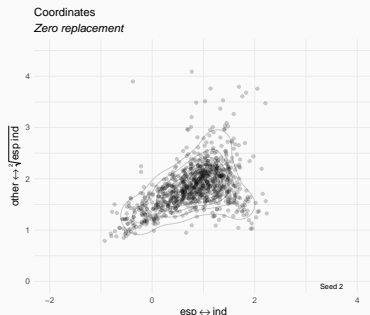
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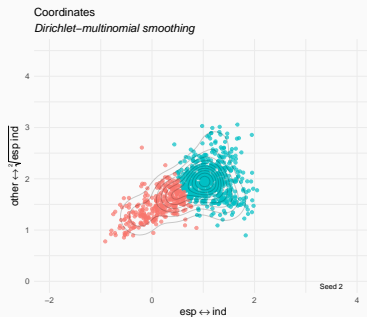
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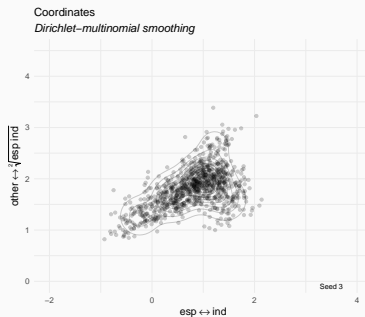
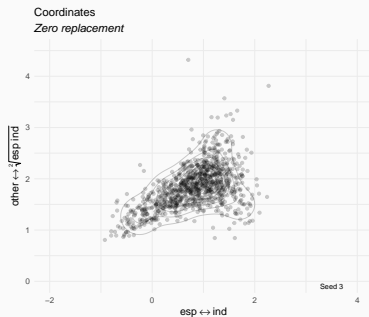
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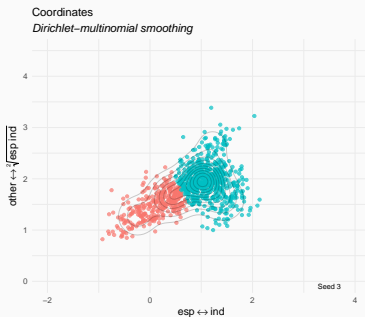
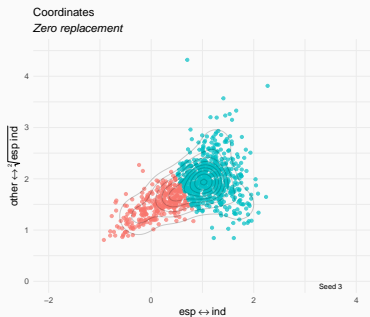
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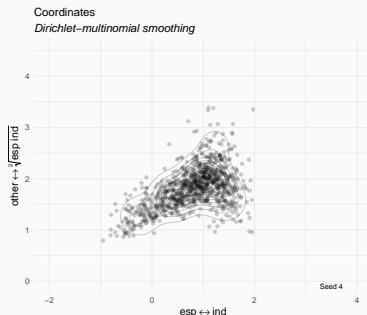
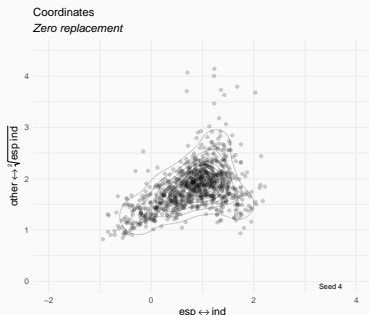
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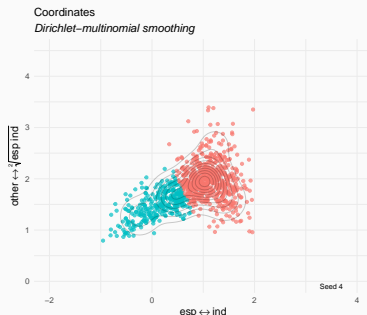
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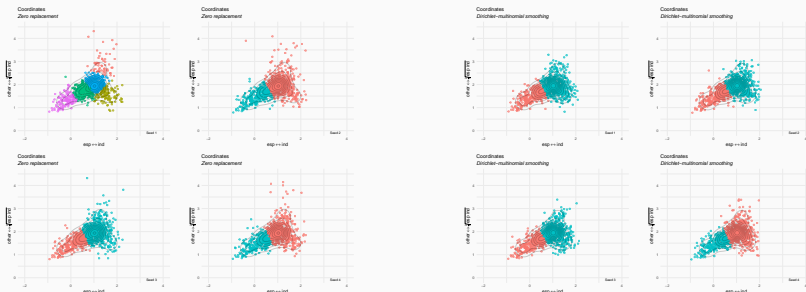


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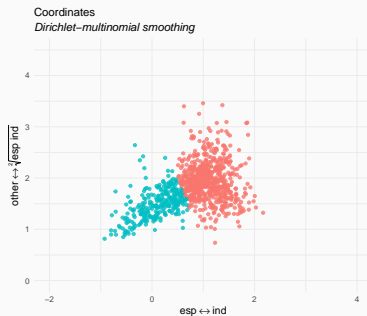
Consensus clustering

- Consensus clustering can be applied to summarise all B clusterings.
→ Majority voting (Dudoit and Fridlyand, 2003)).



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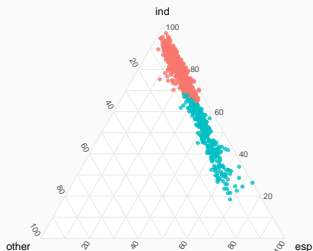
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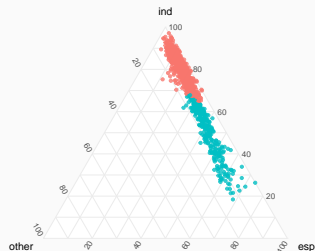
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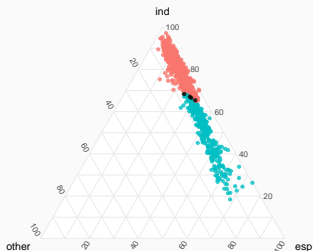
Dirichlet-multinomial smoothing



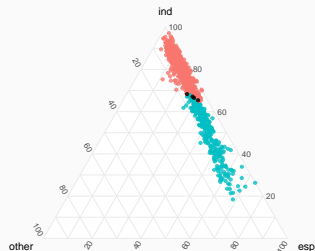
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→ Majority voting (Dudoit and Fridlyand, 2003)).
- Only *four* municipalities differ in the final clustering.

Zero replacement



Dirichlet-multinomial smoothing



Final remarks

- An approach to cluster count data when only the relative relation between parts is of interest has been presented.
- A parametric approach can be constructed in such a way that the variability coming from a multinomial counting process can be incorporated to the observed compositional variability.
- To obtain a final clustering, consensus clustering algorithms can be applied to clustering obtained from each sample.