# Semi-supervised clustering via Markov Aggregation

*Poster presentation:*

SAC'22, Machine Learning and its Applications Track

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on April 27, 2022

# » Content

## Introduction

* Unsupervised clustering
* Semi-supervised clustering

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* Unsupervised clustering
* Semi-supervised clustering

# » Unsupervised clustering

Given:

# » Unsupervised clustering

Given:

* Set of unlabeled data points

# » Unsupervised clustering

Given:

* Set of unlabeled data points

Aim:

# » Unsupervised clustering

Given:

- Set of unlabeled data points

Aim:

- Group data points based on some "similarity" measure

## Introduction

* Unsupervised clustering
* Semi-supervised clustering

# » Semi-supervised clustering

Prior information:

# » Semi-supervised clustering

Prior information:

* Partition-level side information: labeled data points

# » Semi-supervised clustering

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* Partition-level side information: labeled data points
* Instance-level side information: pairwise constraints

# » Semi-supervised clustering

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* Partition-level side information: labeled data points
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  * must-link constraints

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Prior information:

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* Instance-level side information: pairwise constraints
    * must-link constraints
    * cannot-link constraints

## Semi-Supervised Clustering via Markov Aggregation

* Markov Aggregation
* Clustering via Markov Aggregation
* Algorithm

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# » Markov Aggregation

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* Markov chain $\mathbf{X} \sim \mathrm{Mar}(\mathcal{X}, \mathbb{P})$ on the alphabet $\mathcal{X}$

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How:

* Mapping of $\mathbf{X}$ onto $\mathbf{Y}$ via a
  * deterministic mapping $\rightarrow g\colon \mathcal{X} \rightarrow \mathcal{Y}$

# » Cost function

## Rationale

*The mapping $g$ should achieve that . . .*

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*The mapping $g$ should achieve that . . .*

1. the hidden Markov process $\mathbf{Y}$ is *Markov* &
2. preserves the *temporal dependence structure* of $\mathbf{X}$.

# » Cost function

$$\boxed{\mathcal{C}_\beta(\mathbf{X}, \mathbb{W}) := (1 - 2\beta)\left(H(Y_2|Y_1) - H(Y_2|X_1)\right) - \beta I(Y_1; Y_2)}$$

Rana Ali Amjad, Clemens Blochl, and Bernhard C. Geiger. "A Generalized Framework For Kullback–Leibler Markov Aggregation". In: *IEEE Transactions on Automatic Control* 65.7 (July 2020), pp. 3068–3075. ISSN: 2334-3303. DOI: 10.1109/tac.2019.2945891. URL: http://dx.doi.org/10.1109/TAC.2019.2945891

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- $\beta = 1$: *information bottleneck problem*

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## Semi-Supervised Clustering via Markov Aggregation

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# » Clustering via Markov Aggregation

Introduction

Idea:

## » Clustering via Markov Aggregation



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* Minimizing the cost function $\rightarrow$ grouping of states $\mathbf{X}$

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$$P_{i \to j} \propto \mathrm{e}^{-\frac{\|x_i - x_j\|_2^2}{\sigma_k}}$$

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* $\sigma_k$ . . . . . . scaling parameter

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# » Semi-supervised sequential algorithm

## Visualization

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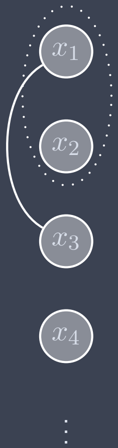
## Visualization



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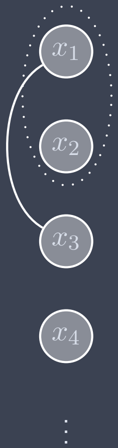


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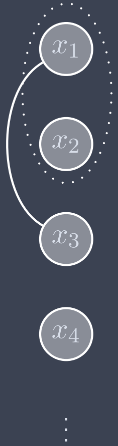


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* Initial aggregation function $g_{init} \longrightarrow$ *greedy coloring algorithm*

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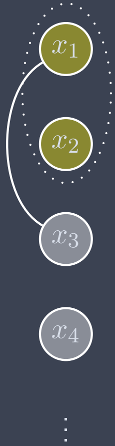


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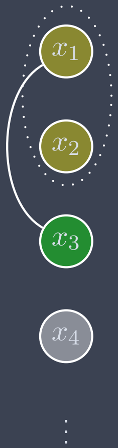


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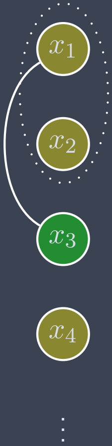


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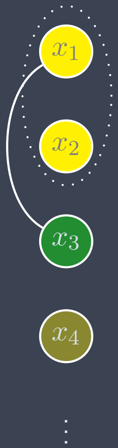

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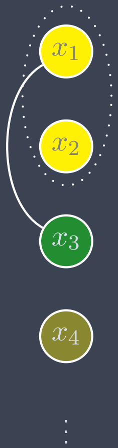


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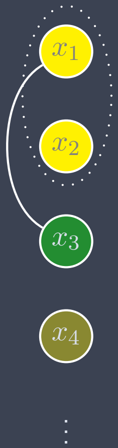


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$y_2$ *not allowed*

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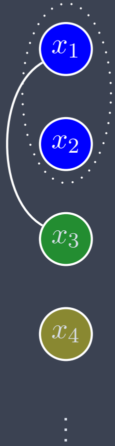


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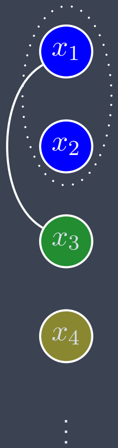


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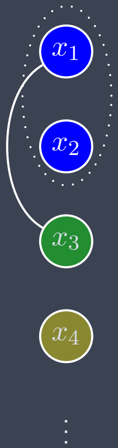


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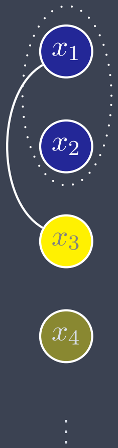

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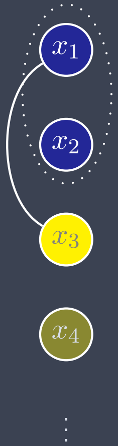


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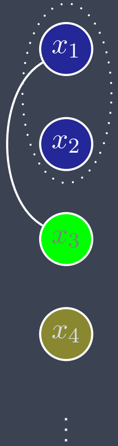


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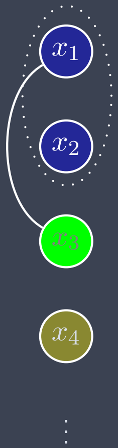


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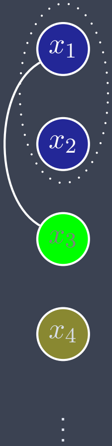


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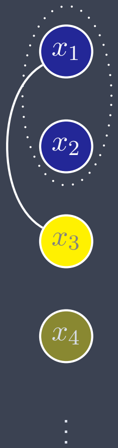


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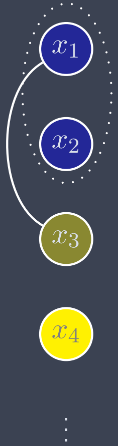

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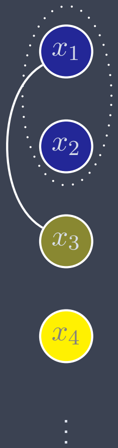


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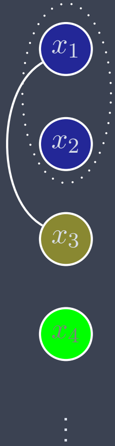


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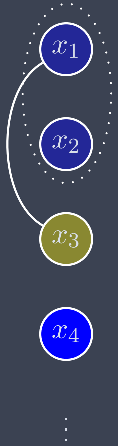


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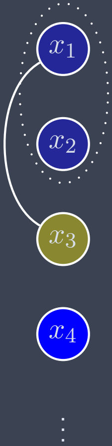


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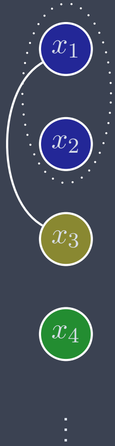


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## Experiments

* Experimental setup
* Influence of the hyperparameters
* Side-information
* Few labeled classes

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Normalized Mutual Information:

$$\mathsf{NMI}(\mathcal{X},\mathcal{Y}) = \frac{2I(\mathcal{Y};\mathcal{X})}{H(\mathcal{Y})+H(\mathcal{X})}$$

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* NMI $= 0$: *no mutual information*
* NMI $= 1$: *identical partitions*

# » Side-information

Pairwise constraints:

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* Select a fraction of data points:

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* Select a fraction of data points:
  - ⇒ Assign the true label

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Pairwise constraints:

- Select a fraction of data points:
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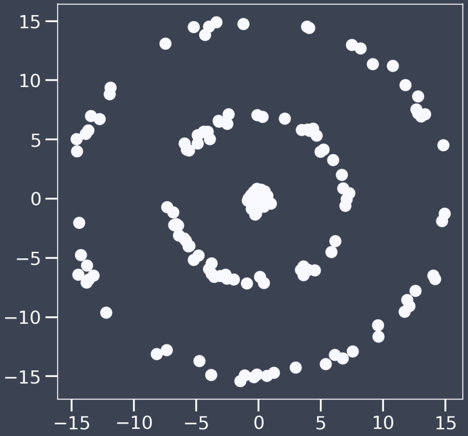
Pairwise constraints:

* Select a fraction of data points:
  * ⇒ Assign the true label
  * ⇒ Generation of pairwise constraints
* Average resulting NMI over 10 runs

# » Side-information

## Unsupervised Clustering



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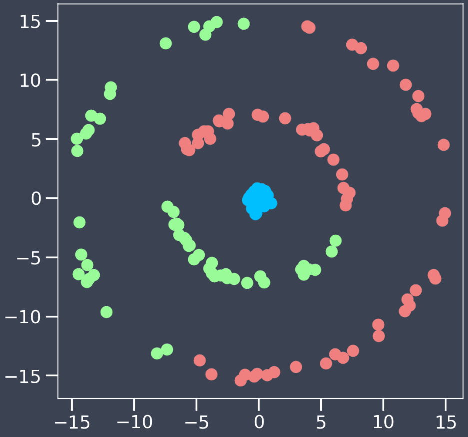

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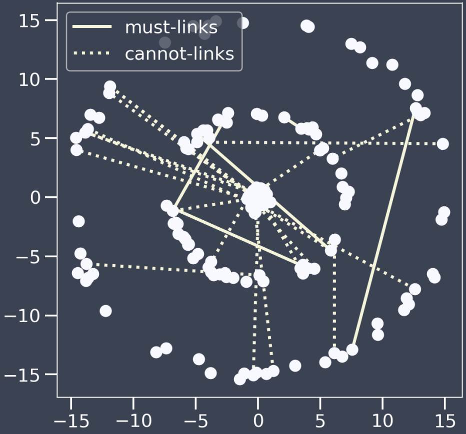
## Semisupervised Clustering



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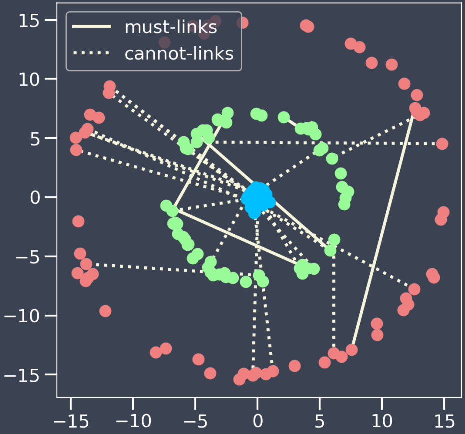

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# » Influence of k

Setup

Setup:

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* Parameters: $\beta = \{0, 0.5, 1\}$, $k$ varied

# » Influence of k

Setup

Setup:

- Parameters: $\beta = \{0, 0.5, 1\}$, $k$ varied
- Fraction of labeled data: 0, 10, 20, 30%

# » Influence of k

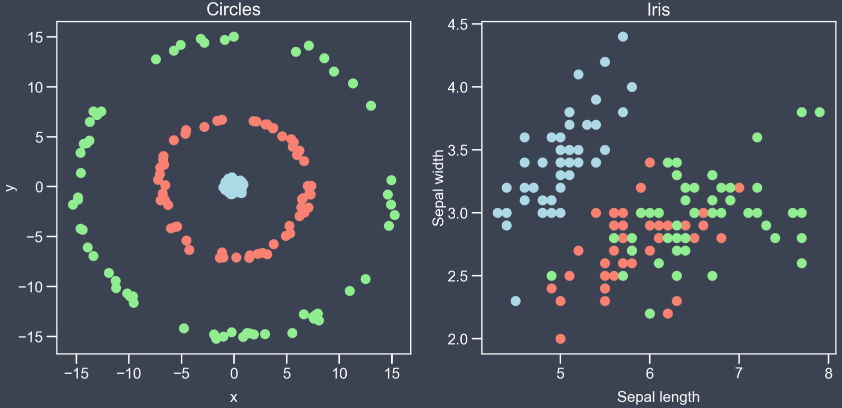
Setup

Setup:

- Parameters: $\beta = \{0, 0.5, 1\}$, $k$ varied
- Fraction of labeled data: 0, 10, 20, 30%
- Datasets: circles, iris

# » Influence of k

## Setup



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Setup

Setup:

* Parameters: $\beta = \{0, 0.5, 1\}$, $k$ varied
* Fraction of labeled data: 0, 10, 20, 30%
* Datasets: circles, iris

Observations:

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Results: Circles dataset

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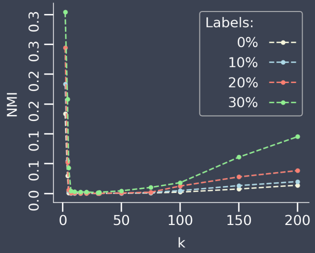
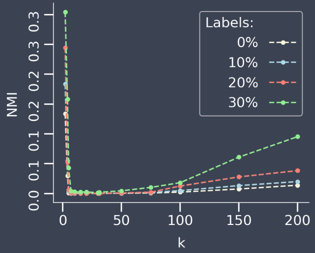



$\beta = 0$

# » Influence of k

## Results: Circles dataset

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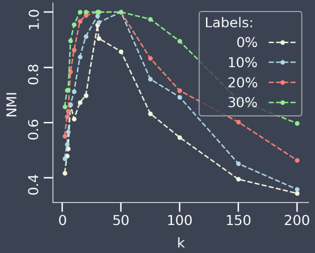


$\beta = 0.5$

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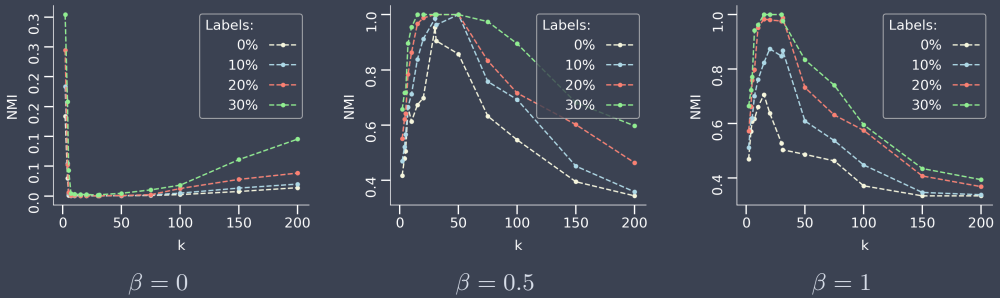
## Results: Circles dataset



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Results: Iris dataset

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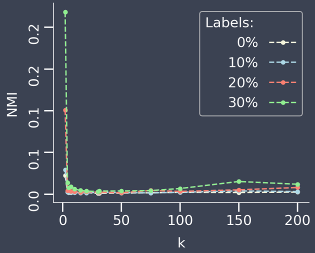
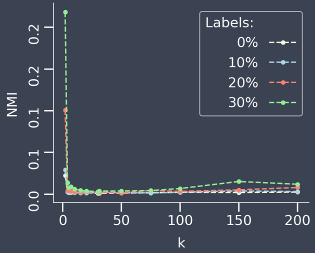


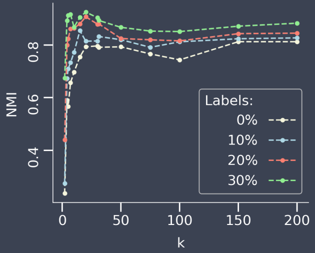

$\beta = 0$

# » Influence of k

## Results: Iris dataset




$\beta = 0$




$\beta = 0.5$

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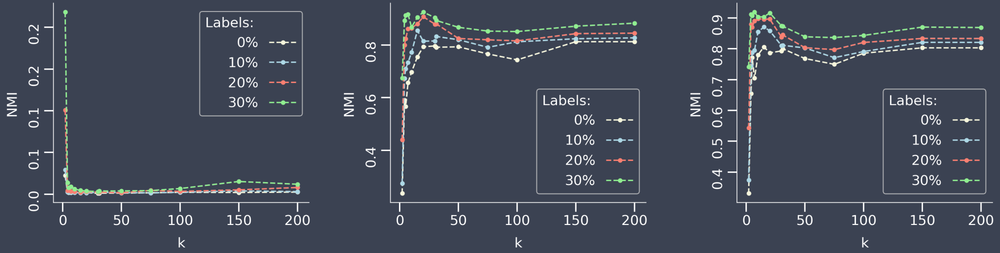


$\beta = 0$ $\beta = 0.5$ $\beta = 1$

# » Influence of beta

Setup

Setup:

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Setup

Setup:

* Parameters: $k = 20$, $\beta$ varied

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Setup:

* Parameters: $k = 20$, $\beta$ varied
* Datasets: selected UCI datasets

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Observations:

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Setup:

* Parameters: $k = 20$, $\beta$ varied
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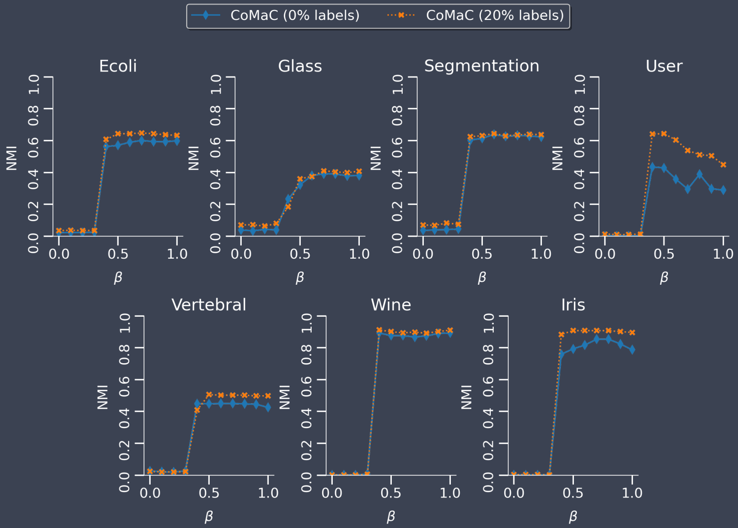
Observations:

* Influence on accuracy for *unsupervised* and *semi-supervised* case

# » Influence of beta

## Results: semi-supervised (20% labeled data)



## Experiments

* Experimental setup
* Influence of the hyperparameters
* Side-information
* Few labeled classes

# » Side-information



Setup:

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Setup

Setup:

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[1] Marek Smieja and Bernhard C. Geiger. "Semi-supervised cross-entropy clustering with information bottleneck constraint". In: *Information Sciences* 421 (Dec. 2017), pp. 254–271

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Setup:

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* Comparison to state-of-the-art-algorithms [1]

[1] Smieja and Geiger, "Semi-supervised cross-entropy clustering with information bottleneck constraint"

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Observations:

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* Performance compared to other methods

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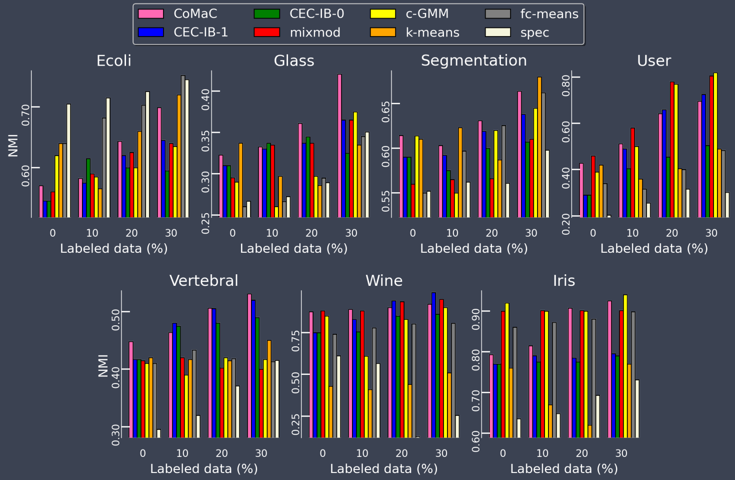
# » Side-information

## Results: Overview



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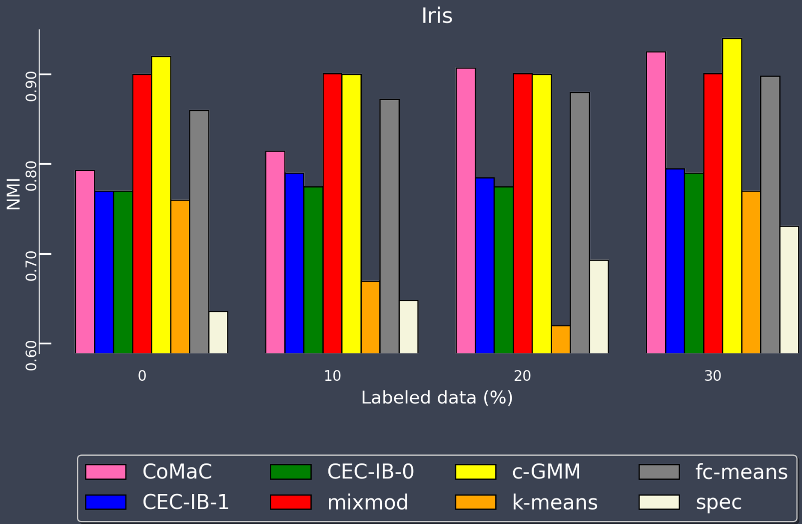
## Results: Details



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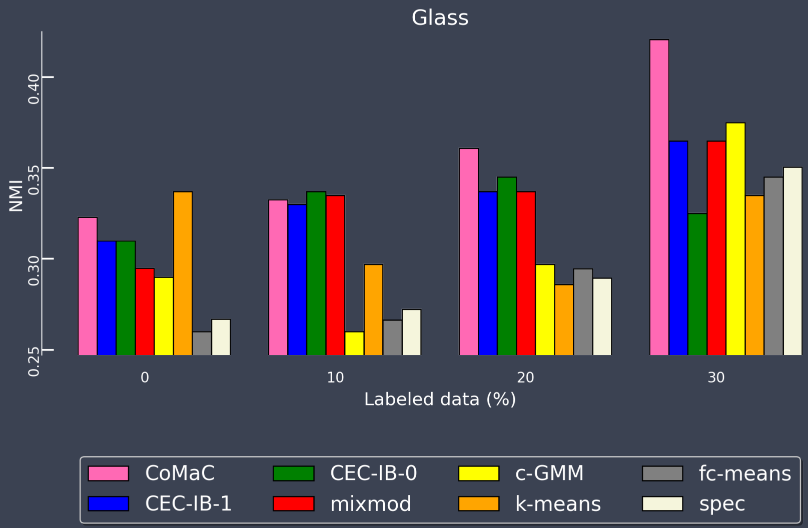

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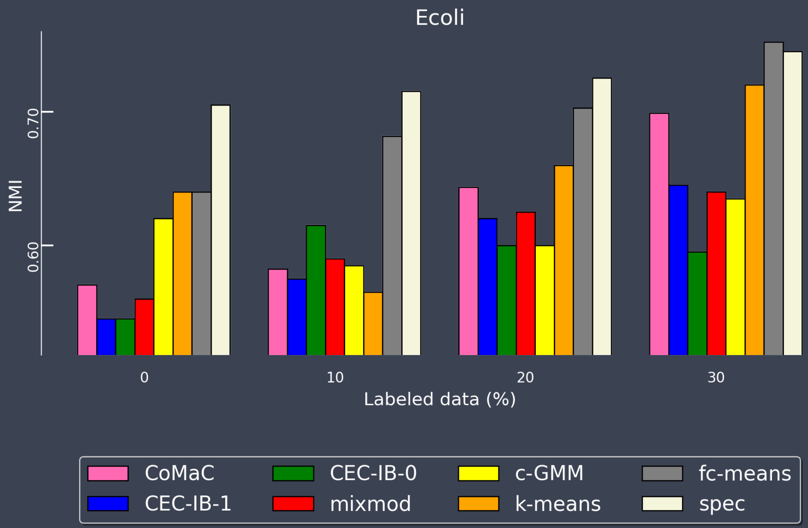

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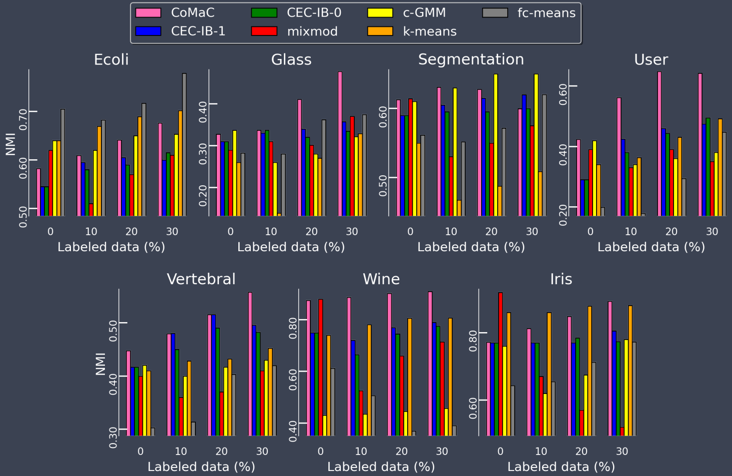
## Results: Few vs all classes



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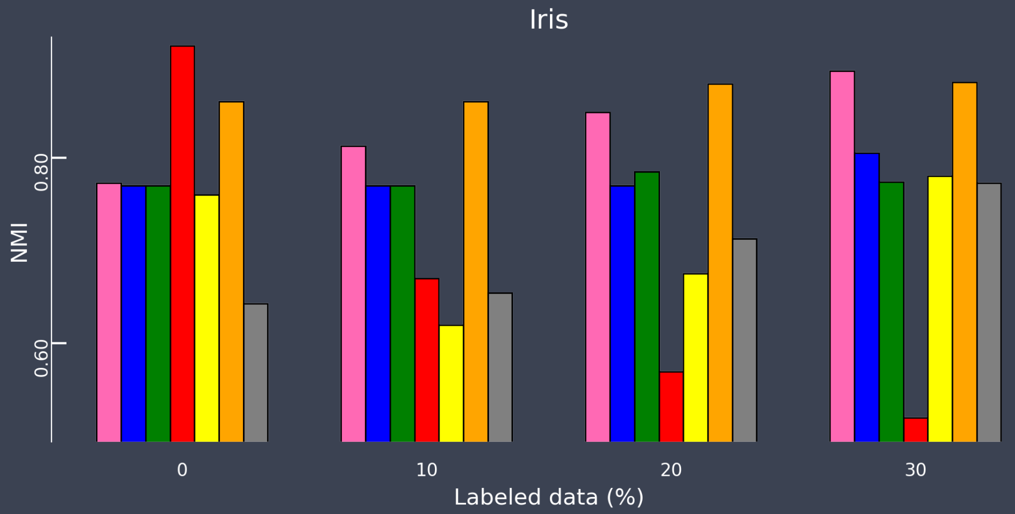

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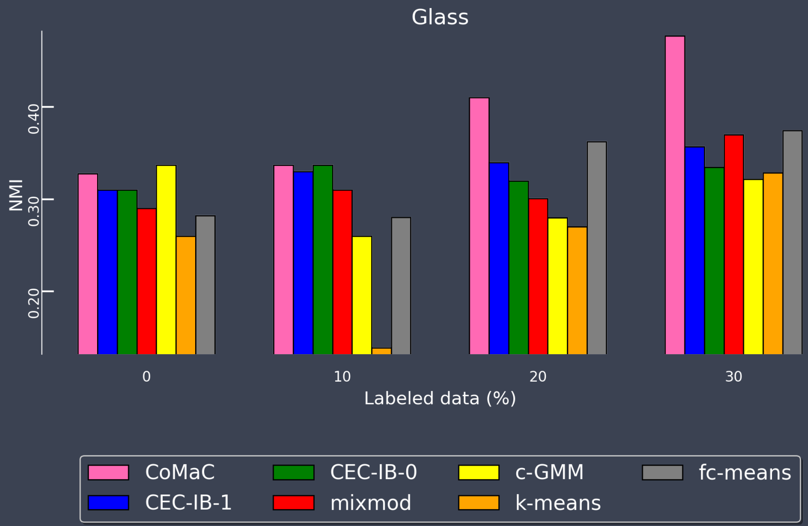

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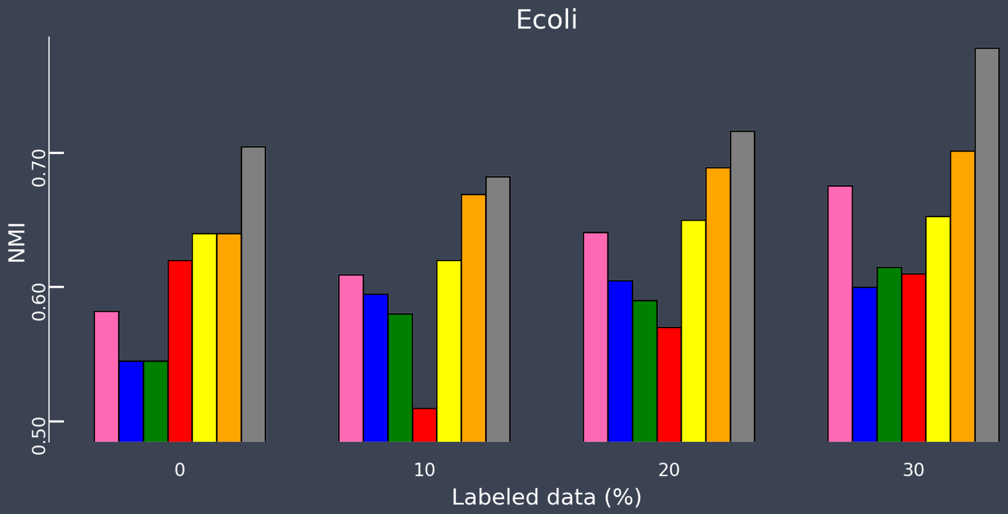

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  - Problem for few classes: constrained data pairs are forced to stay in place

# Conclusion

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Full-text: `https://arxiv.org/abs/2112.09397`

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</> `https://github.com/stegsoph/Constrained-Markov-Clustering.git`

Thank you for your attention!