Conditional tSNE

Bo Kang   Jefrey Lijffijt   Tijl De Bie
Darío García García
Raúl Santos-Rodríguez

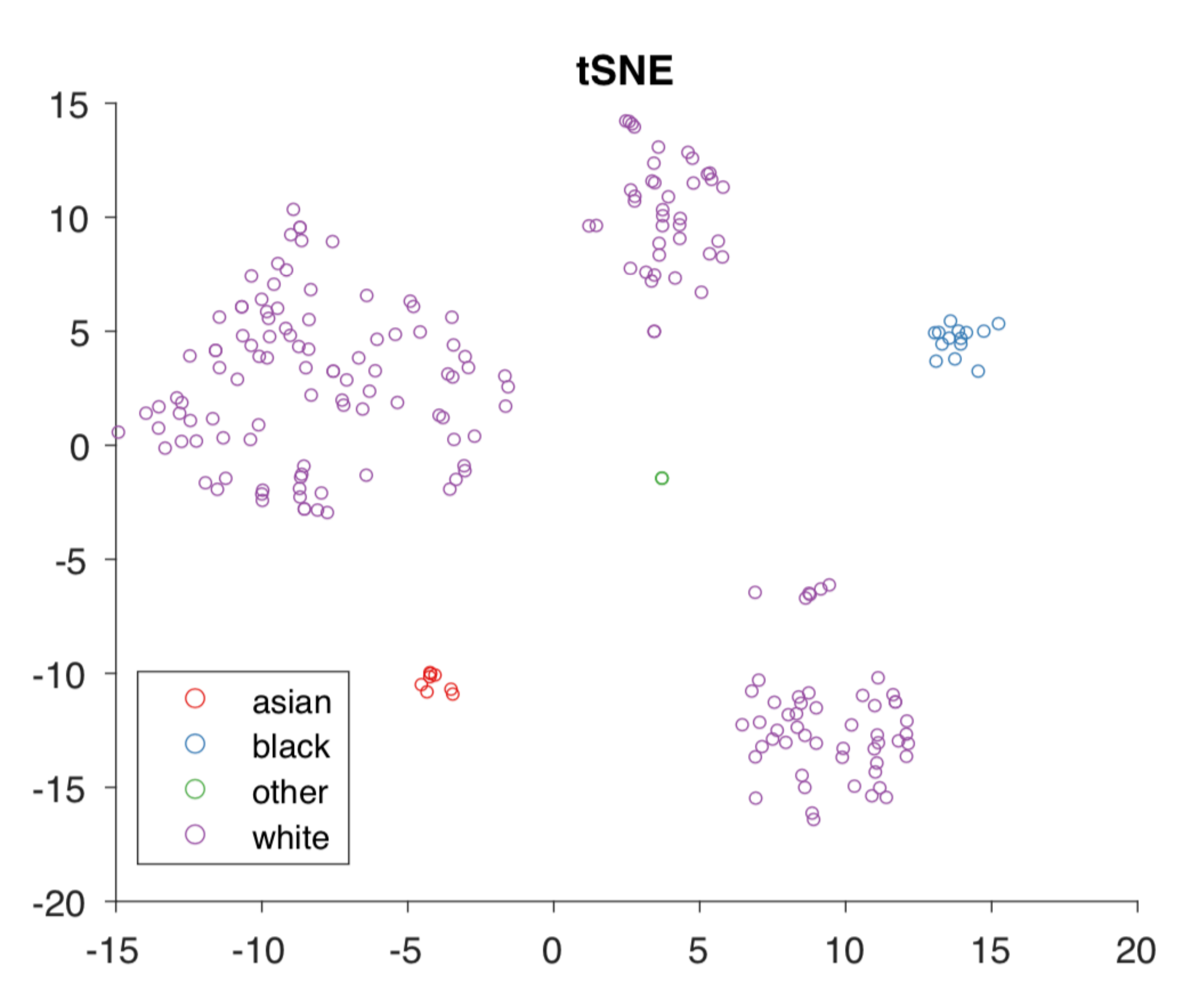
Ghent University
Facebook
University of Bristol

Motivation

- High dim data embeddings often have confounding factors.
- Factors: known, unknown but dominant, sensitive.

Motivation

UCI Adult dataset



Motivation

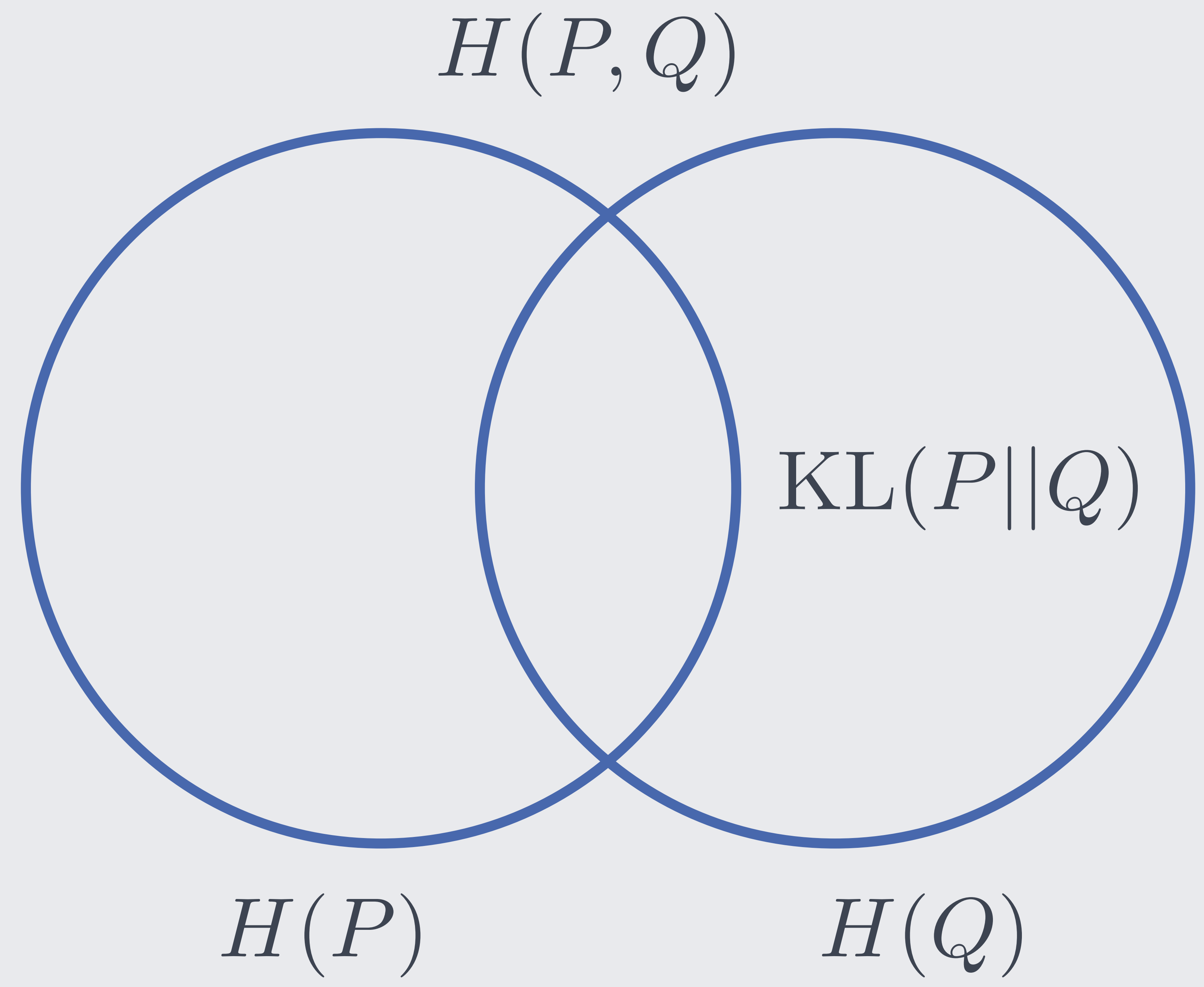
- High dim data embeddings often has confounding factors
- Factors that are known, unknown but dominant, sensitive.
- Find embedding with confounding factors explained away?

Method

tSNE

- High dim proximity P
- Low dim proximity Q
- Objective:

$$\min_{\mathbf{y}} \mathrm{KL}(P||Q)$$



Method

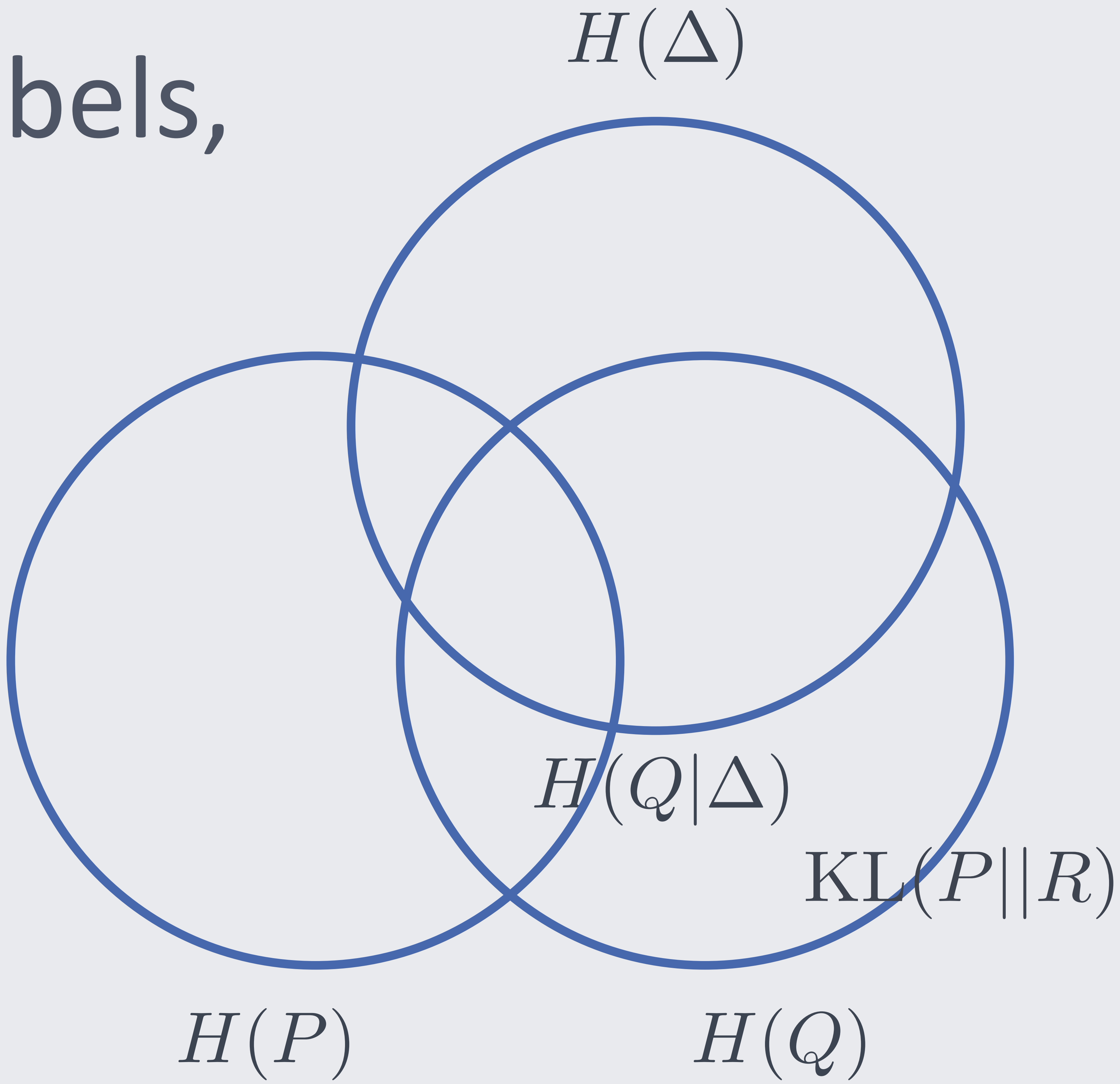
ctSNE

- Confounding factors are encoded by labels, denoted by delta matrix Δ
- Formalize lower dim distribution

$$r_{ij} = P(i, j|\Delta)$$

- Objective:

$$\min_{\mathbf{y}} \mathrm{KL}(P||R)$$



Method

A bit of Bayesian

$$P(i,j) = q_{ij}$$

$$P(\Delta|i,j) = \alpha^{\delta_{ij}} \beta^{1-\delta_{ij}}$$

$$P(\Delta) = \sum_{i \neq j} P(\Delta|i,j) P(i,j)$$

$$P(i,j|\Delta) = \frac{P(\Delta|i,j)P(i,j)}{P(\Delta)} = \frac{\alpha^{\delta_{ij}} \beta^{\delta_{ij}} q_{ij}}{\alpha \sum_{i \neq j : \delta_{ij} = 1} q_{ij} + \beta \sum_{i \neq j : \delta_{ij} = 0} q_{ij}}$$

Method

Intuition tSNE

$$\frac{\partial}{\partial \mathbf{y}_i} \mathrm{KL}(P||Q) \propto \sum_{j \neq i} p_{ij} q_{ij} (\mathbf{y}_i - \mathbf{y}_j) - \sum_{j \neq i} q_{ij}^2 (\mathbf{y}_i - \mathbf{y}_j)$$

Attraction force **Repelling force**

Method

Intuition ctSNE

$$\frac{\partial}{\partial \mathbf{y}_i}\mathrm{KL}(P||R) \propto$$

$$\sum_{j\neq i} p_{ij} q_{ij} (\mathbf{y}_i - \mathbf{y}_j) - \frac{\delta_{ij}\alpha' + (1-\delta_{ij})\beta'}{O} \sum_{j \neq i} q_{ij}^2 (\mathbf{y}_i - \mathbf{y}_j)$$

Attraction force **Weighted repelling force**

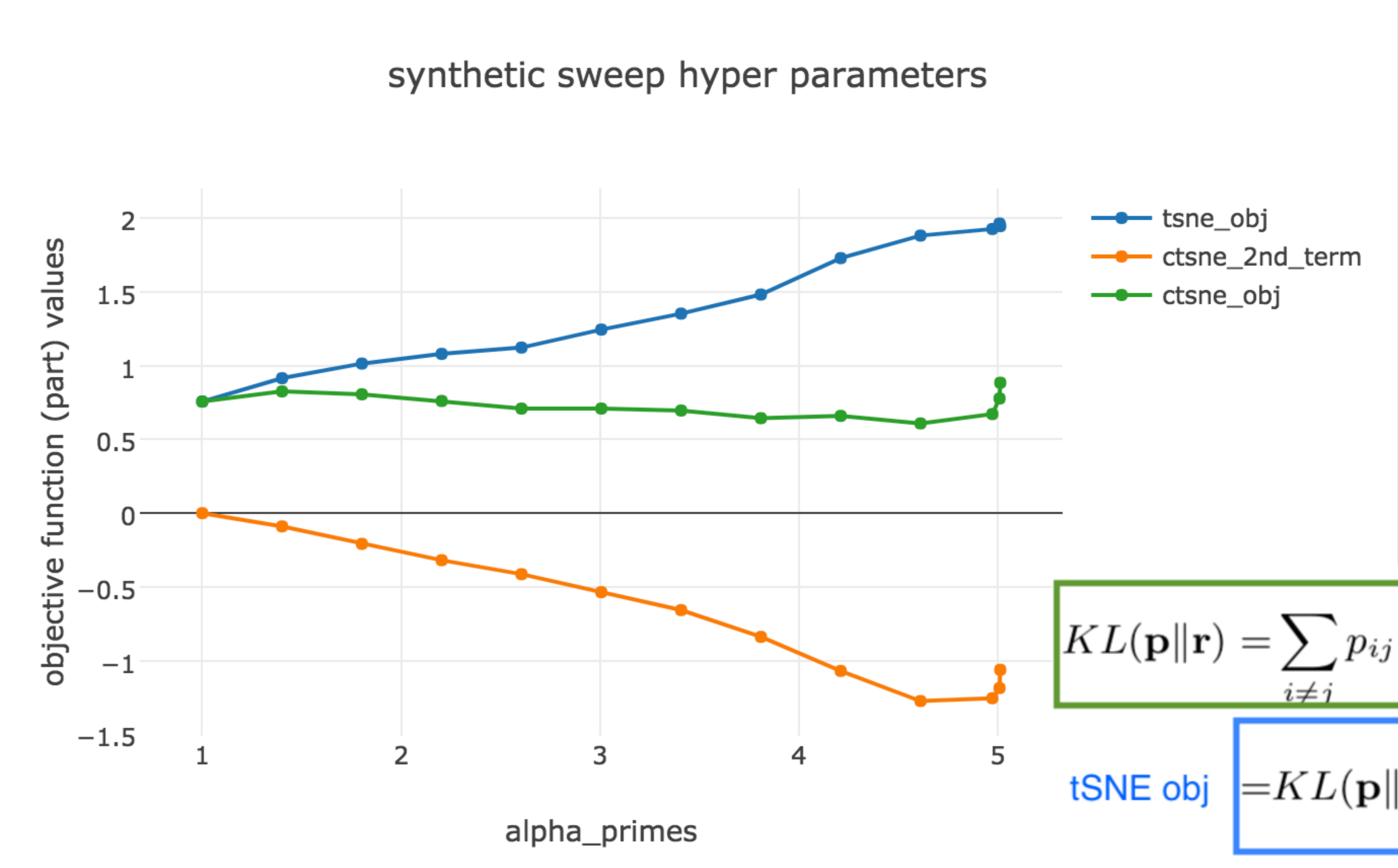
where $O = \alpha' \sum_{i\neq j:\delta_{ij}=1} q_{ij} + \beta' \sum_{i\neq j:\delta_{ij}=0} q_{ij}$

$$1 = \sum_{\Delta} P(\Delta|i,j) = \sum_{\Delta} \alpha^{\delta_{ij}} \beta^{1-\delta_{ij}}$$

$1 = \alpha' \frac{\sum_l n_l(n_l-1)}{n(n-1)} + \beta' \left(1 - \frac{\sum_l n_l(n_l-1)}{n(n-1)}\right)$ where $\alpha' \triangleq \alpha \frac{n!}{\prod_l n_l!}, \ \beta' \triangleq \beta \frac{n!}{\prod_l n_l!}$

Method

Intuition ctSNE ranging alpha



- Label information allows to achieve a closer distribution.

ctSNE obj

$$\boxed{KL(\mathbf{p}\|\mathbf{r}) = \sum_{i\neq j} p_{ij} \log\left(\frac{p_{ij}}{r_{ij}}\right)}$$

tSNE obj

extra term in ctSNE obj

$$\boxed{= KL(\mathbf{p}\|\mathbf{q})} + \boxed{\sum_{i\neq j} p_{ij} \log\left(\frac{\alpha' \sum_{i\neq j:\delta_{ij}=1} q_{ij} + \beta' \sum_{i\neq j:\delta_{ij}=0} q_{ij}}{\alpha'^{\delta_{ij}} \beta'^{1-\delta_{ij}}}\right)},$$

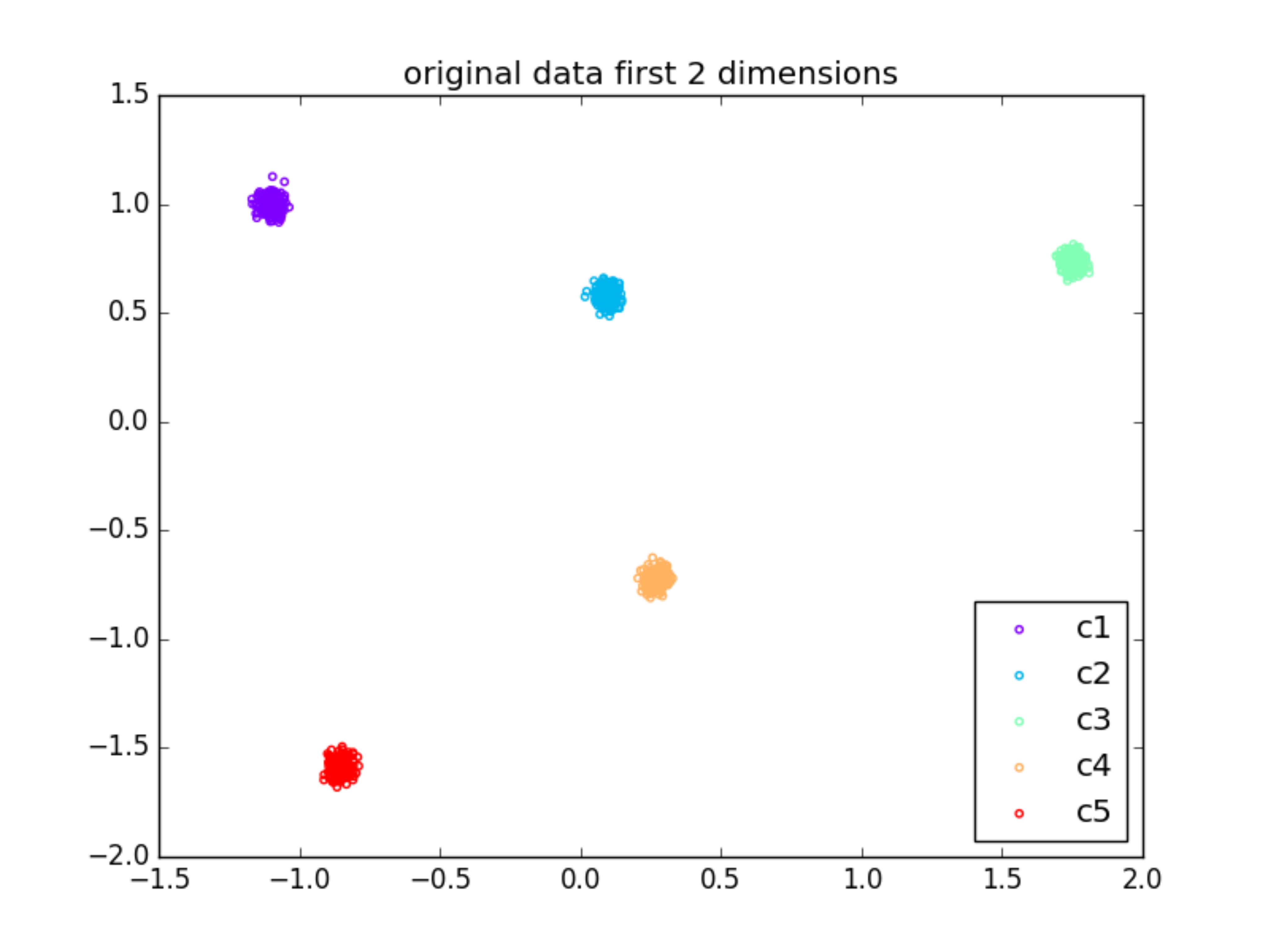
Algorithm

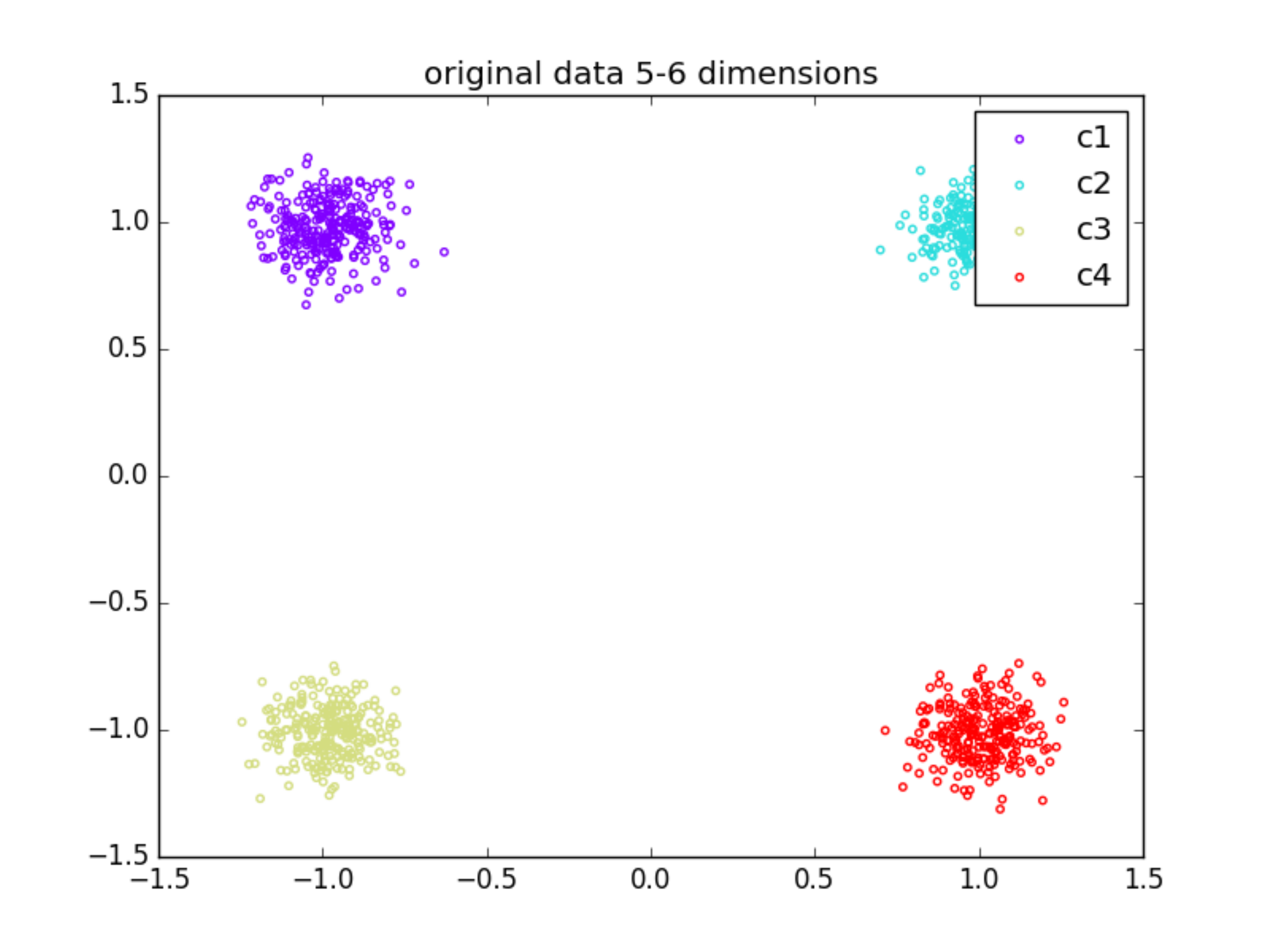
Barnes-Hut approximation

- Exact: $O(n^2)$
- High dim: a vantage-point tree $O(n \log n)$
- Low dim: quad tree $O(n \log n)$
- ctSNE implementation: quad tree with label count.

Experiments

Case study: synthetic dataset





Experiments

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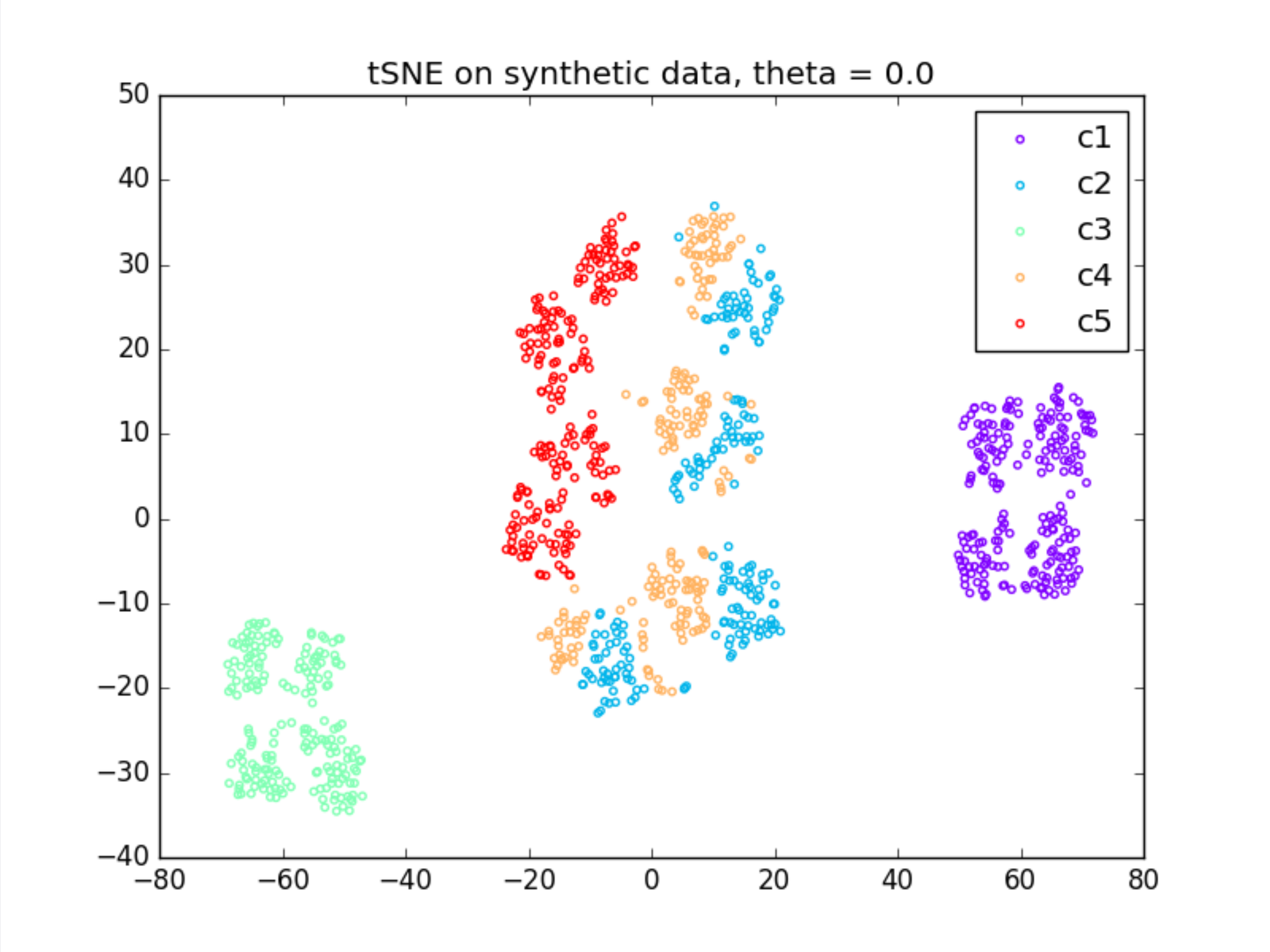

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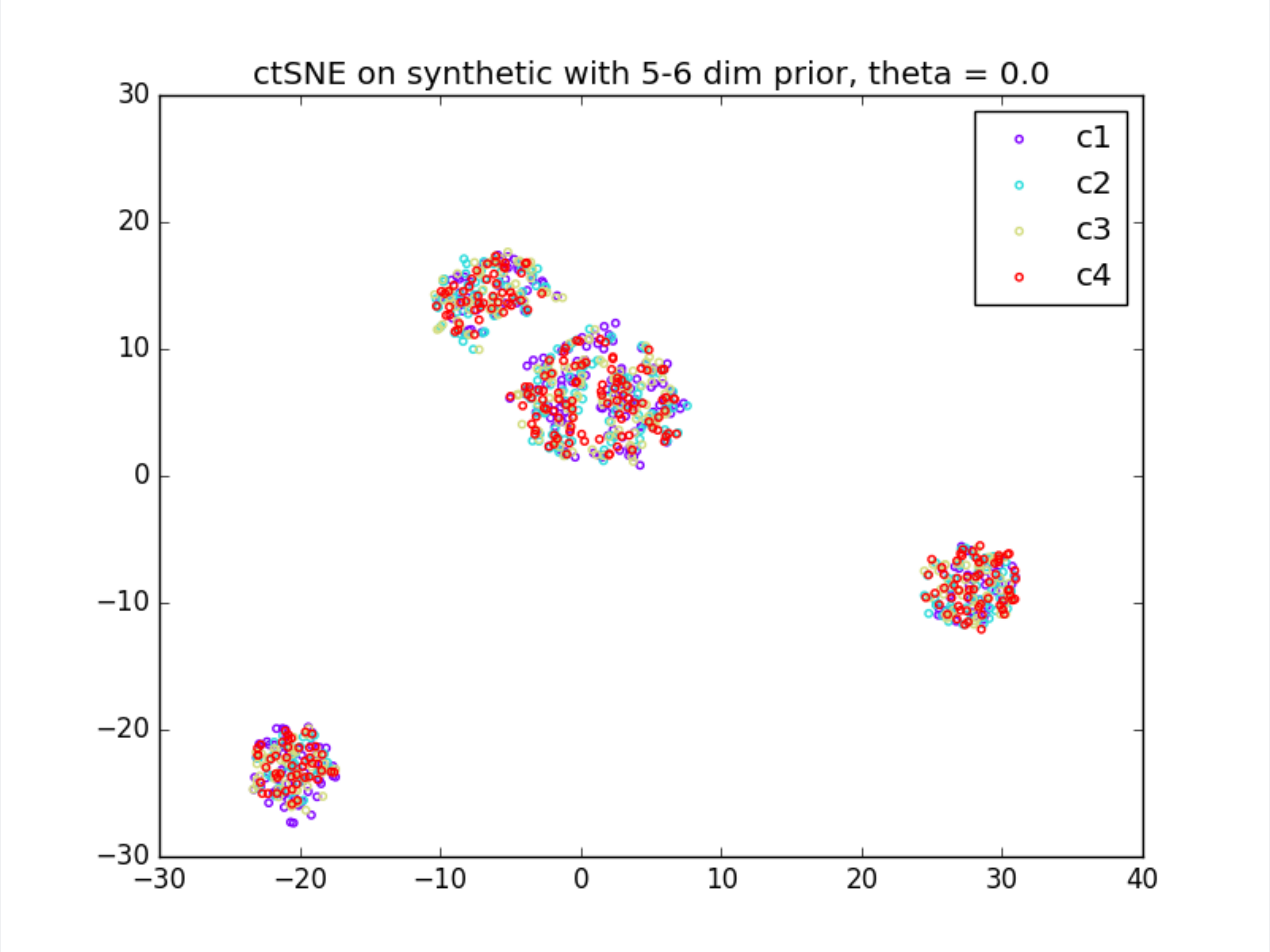

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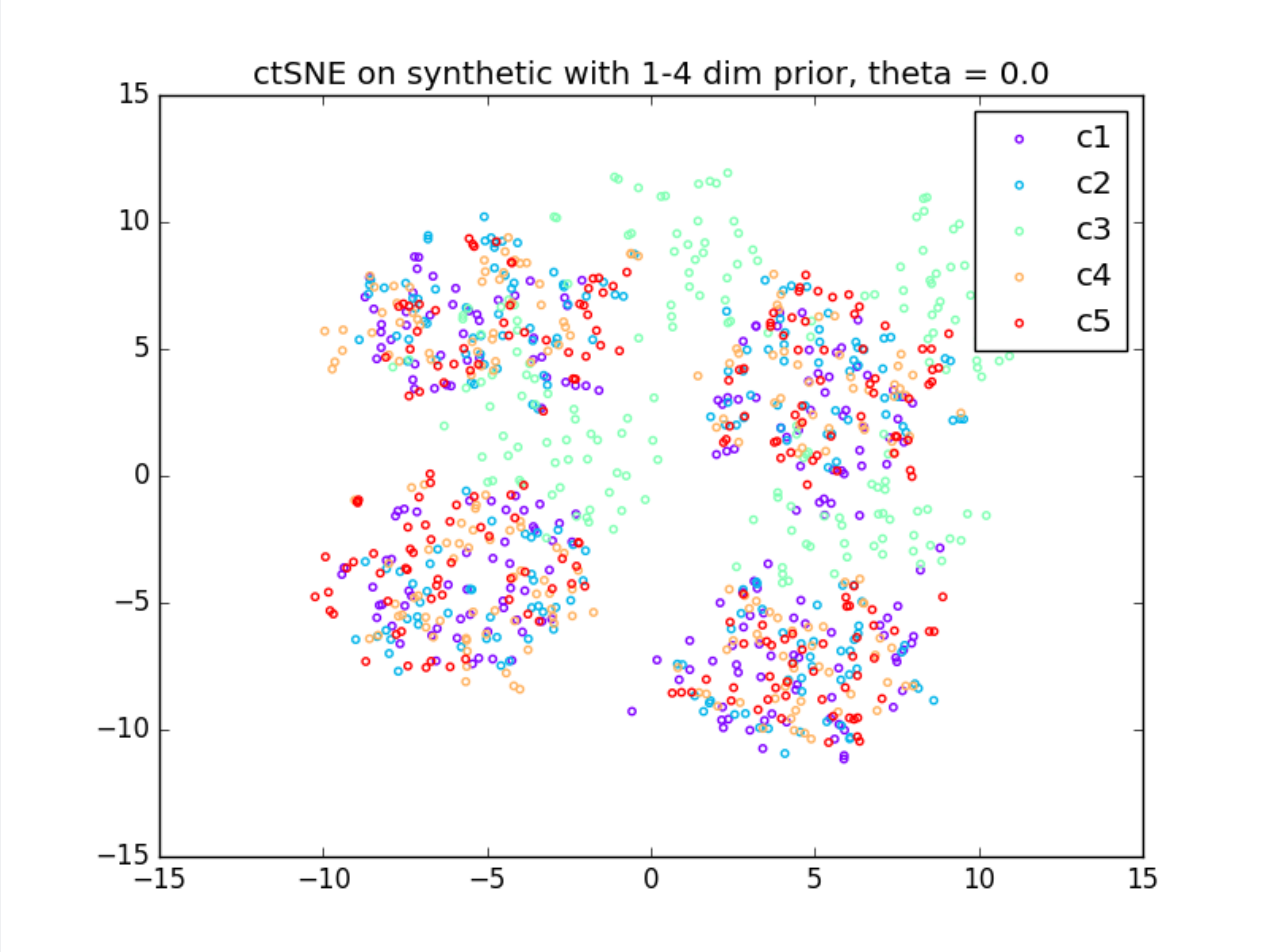

Experiments

Case study: UCI Adult dataset

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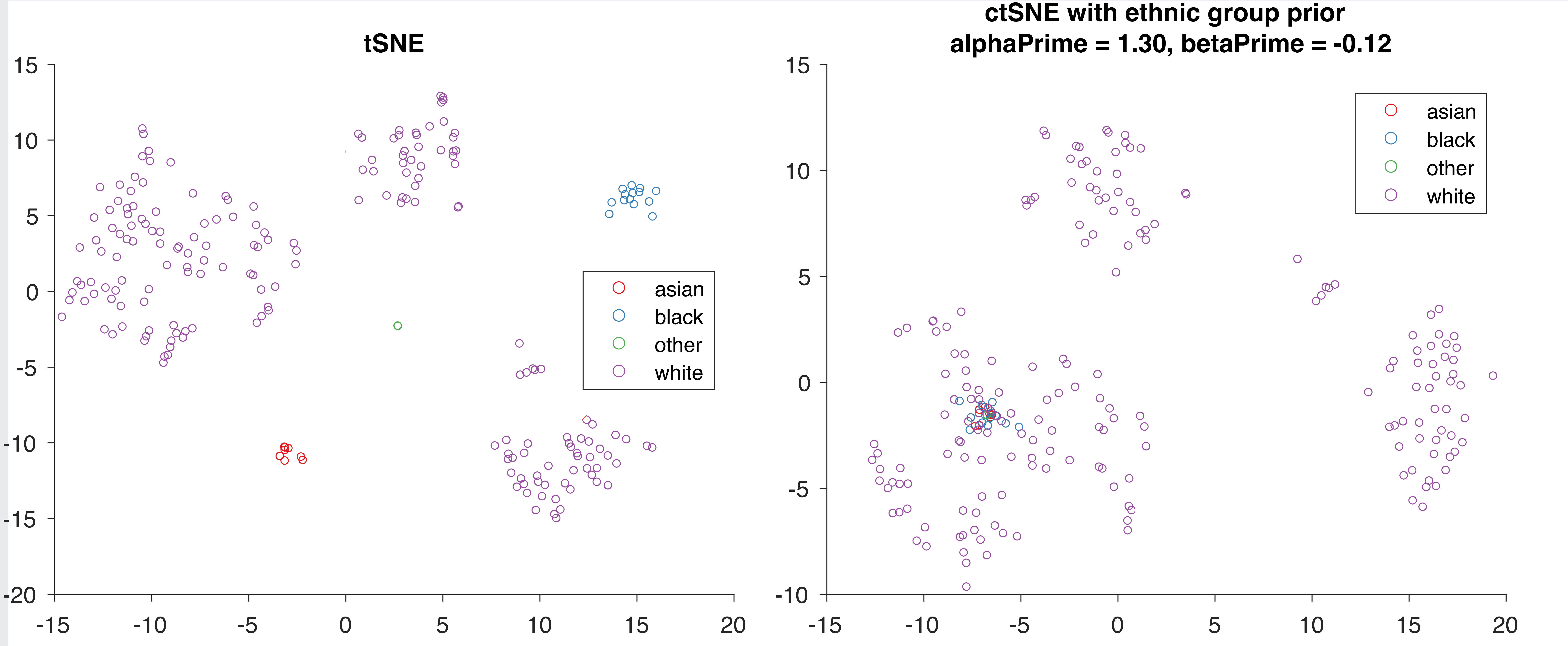

Experiments

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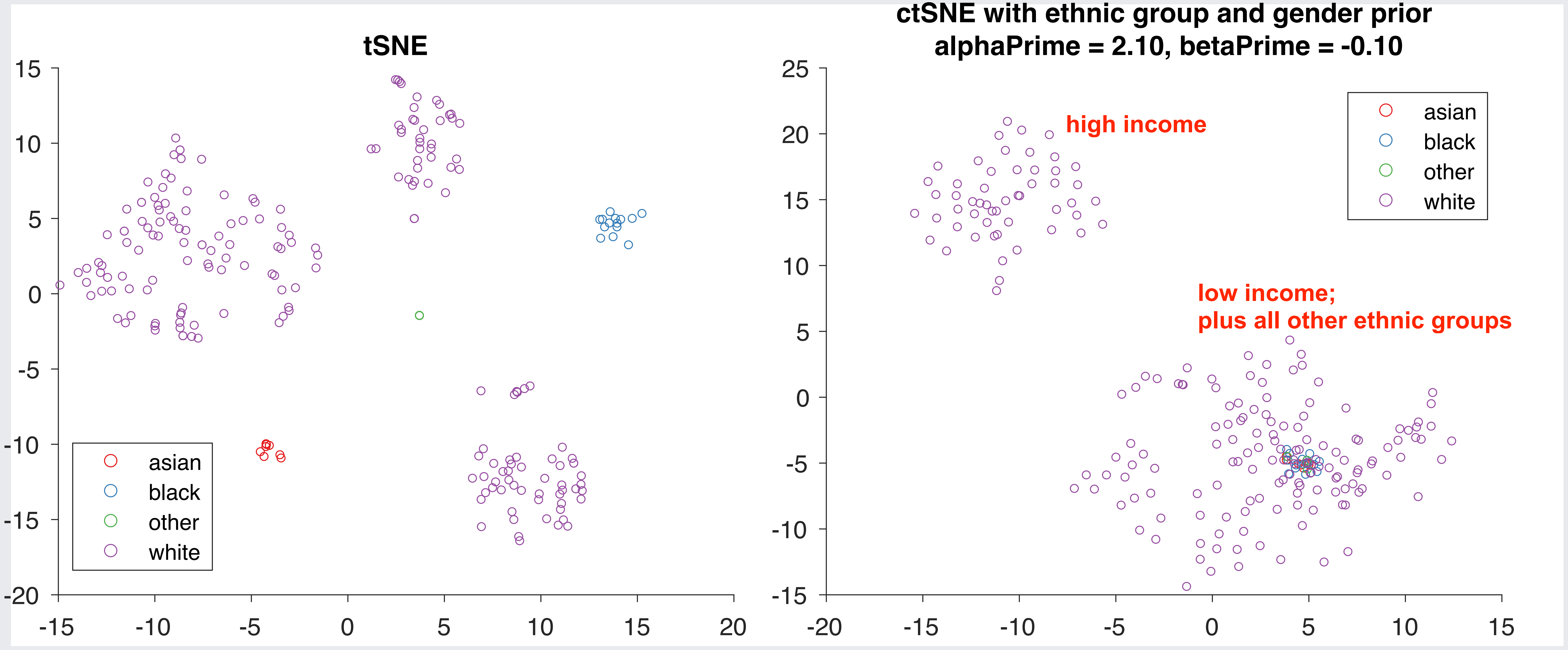


Experiments

Case study: Facebook dataset

- Show me some figures

Experiments

Quantitative benchmark

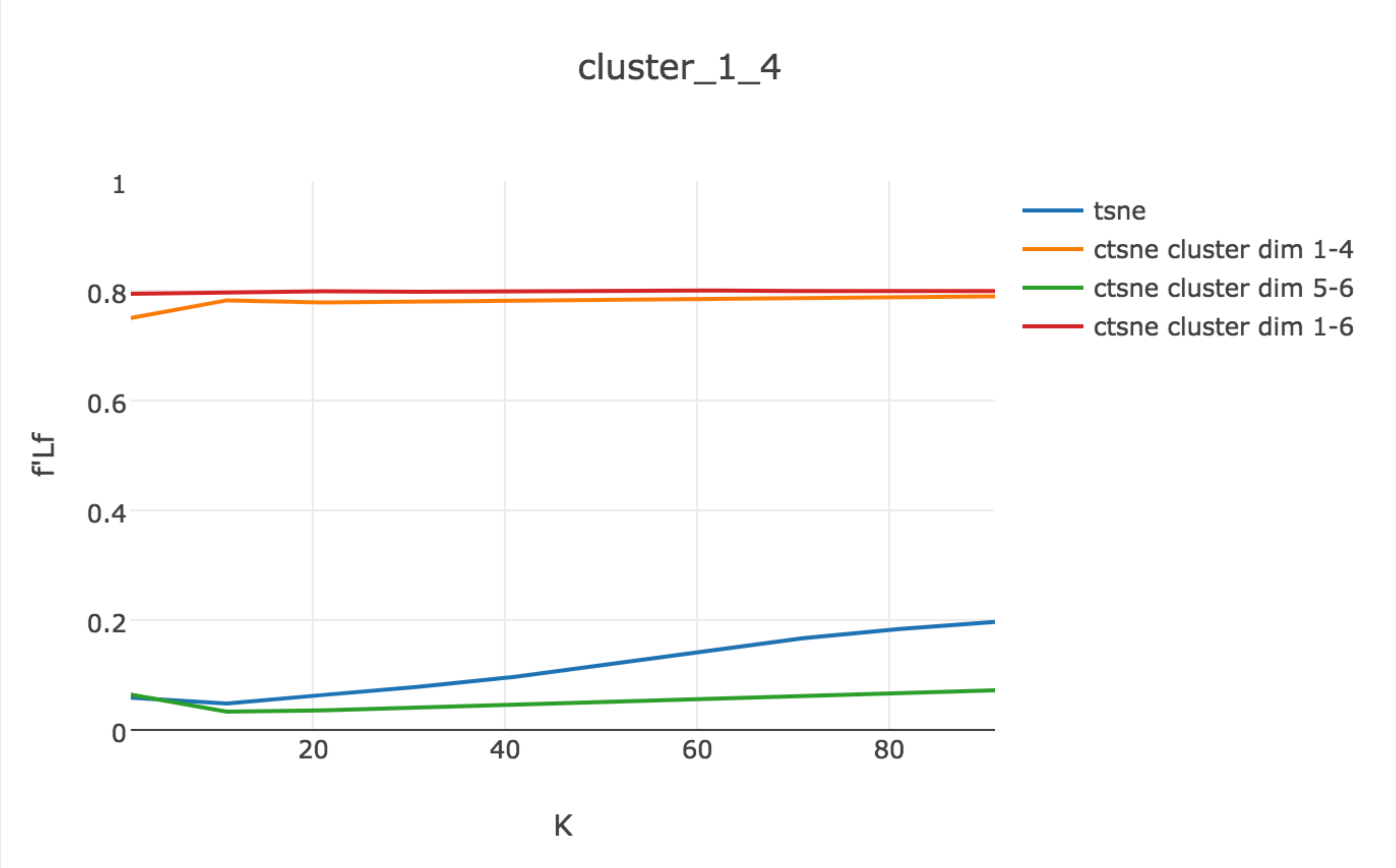
- Construct KNN graph on embedding
- Measure the consistency of a factor over the graph
- Normalized Laplacian score:

$$\mathbf{f}'\mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}\mathbf{f}$$

- Lager the score, less consistent over the graph

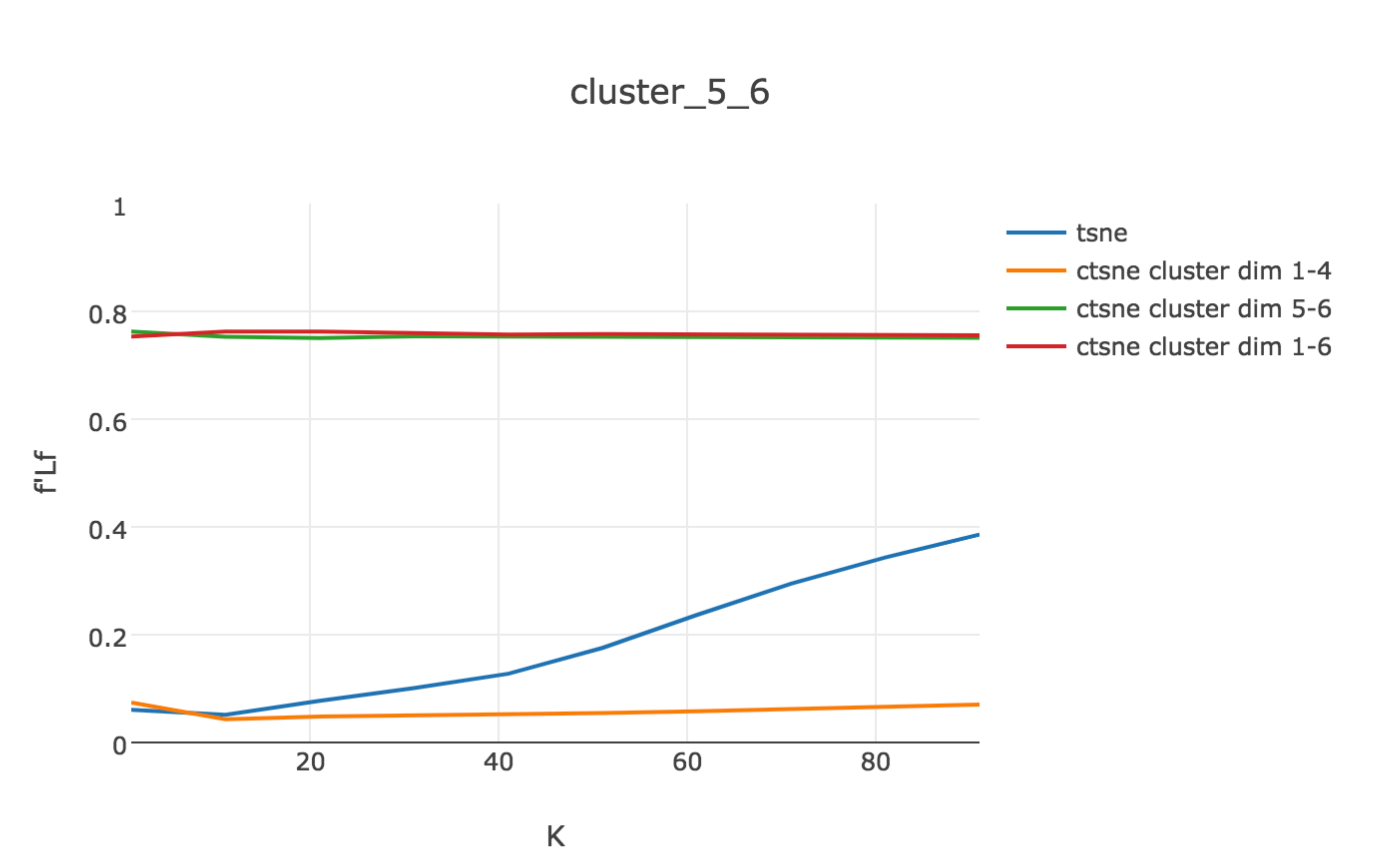
Experiments

Quantitative benchmark



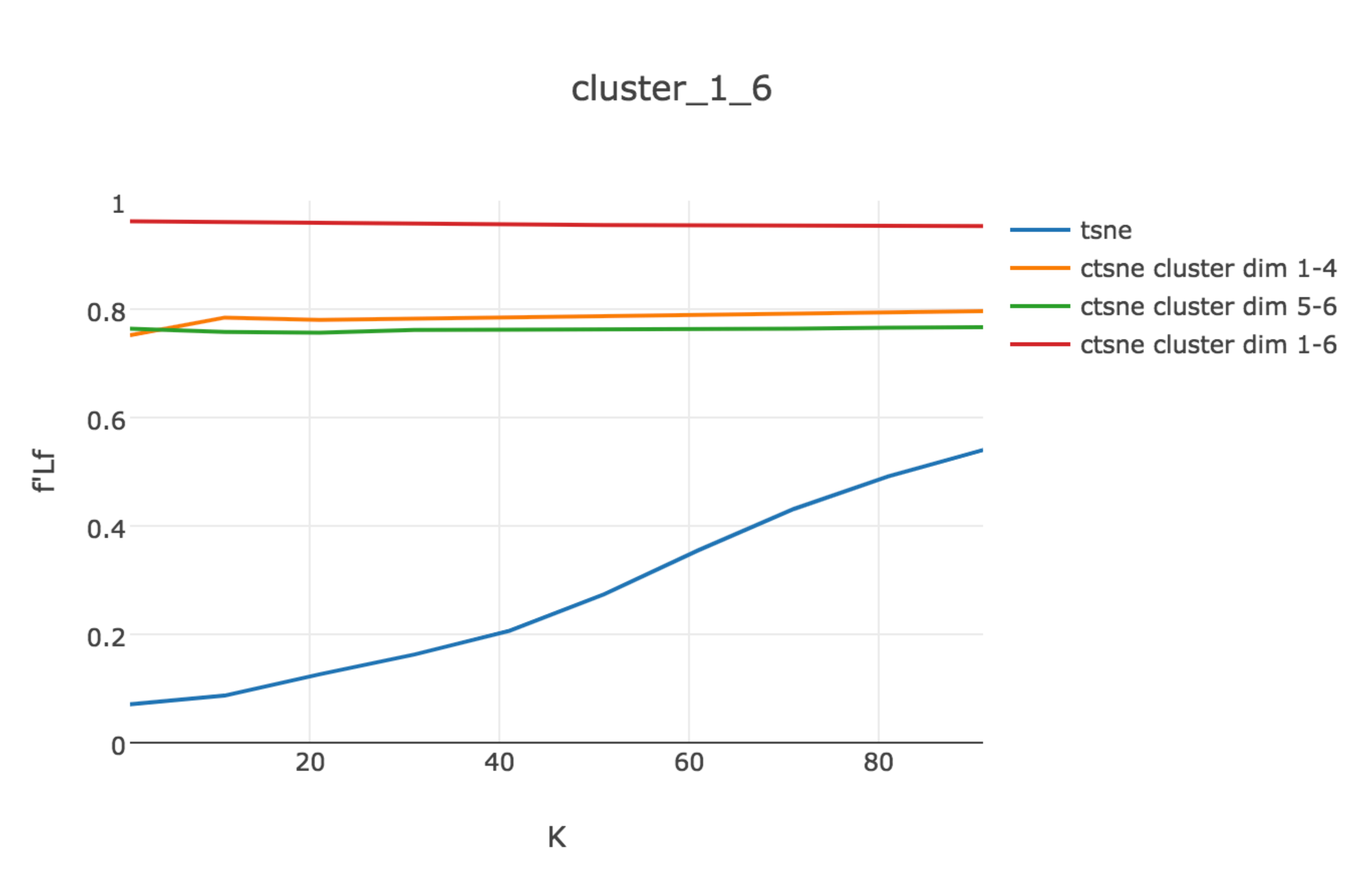
Experiments

Quantitative benchmark



Experiments

Quantitative benchmark



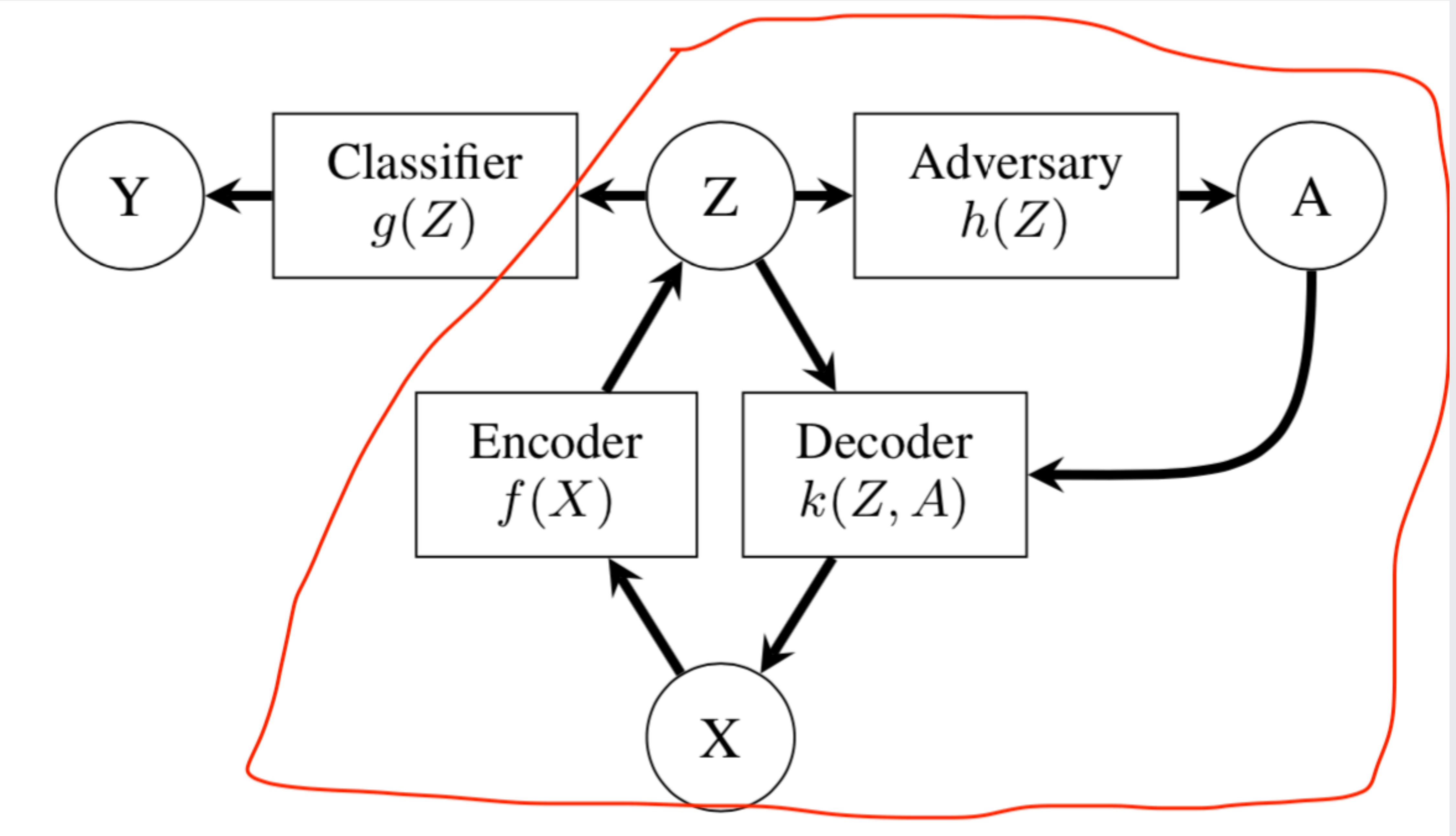
Experiments

Baseline

- Remove label information then apply tSNE
- Example:

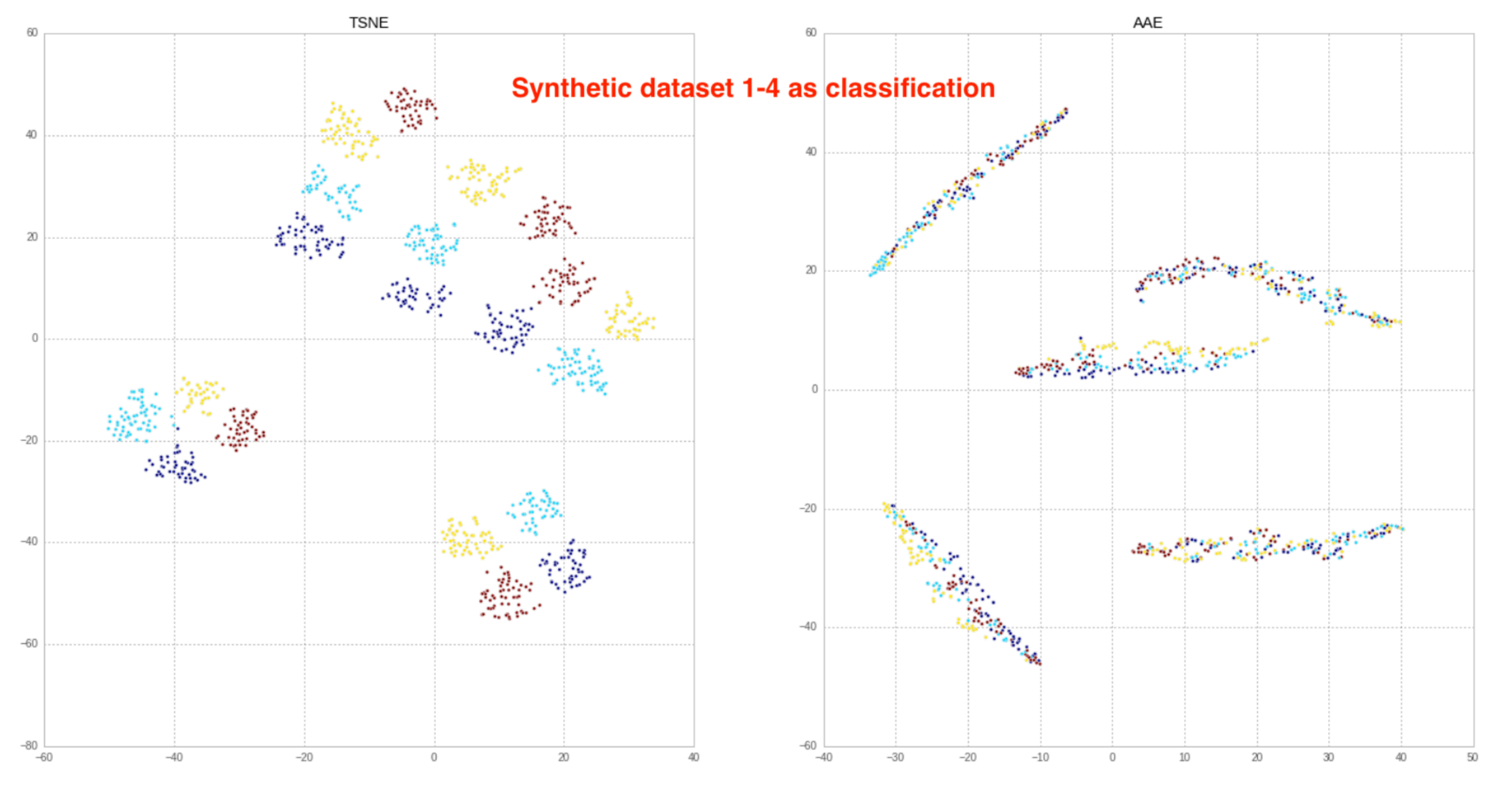
  Adversarial Auto Encoder

  then tSNE



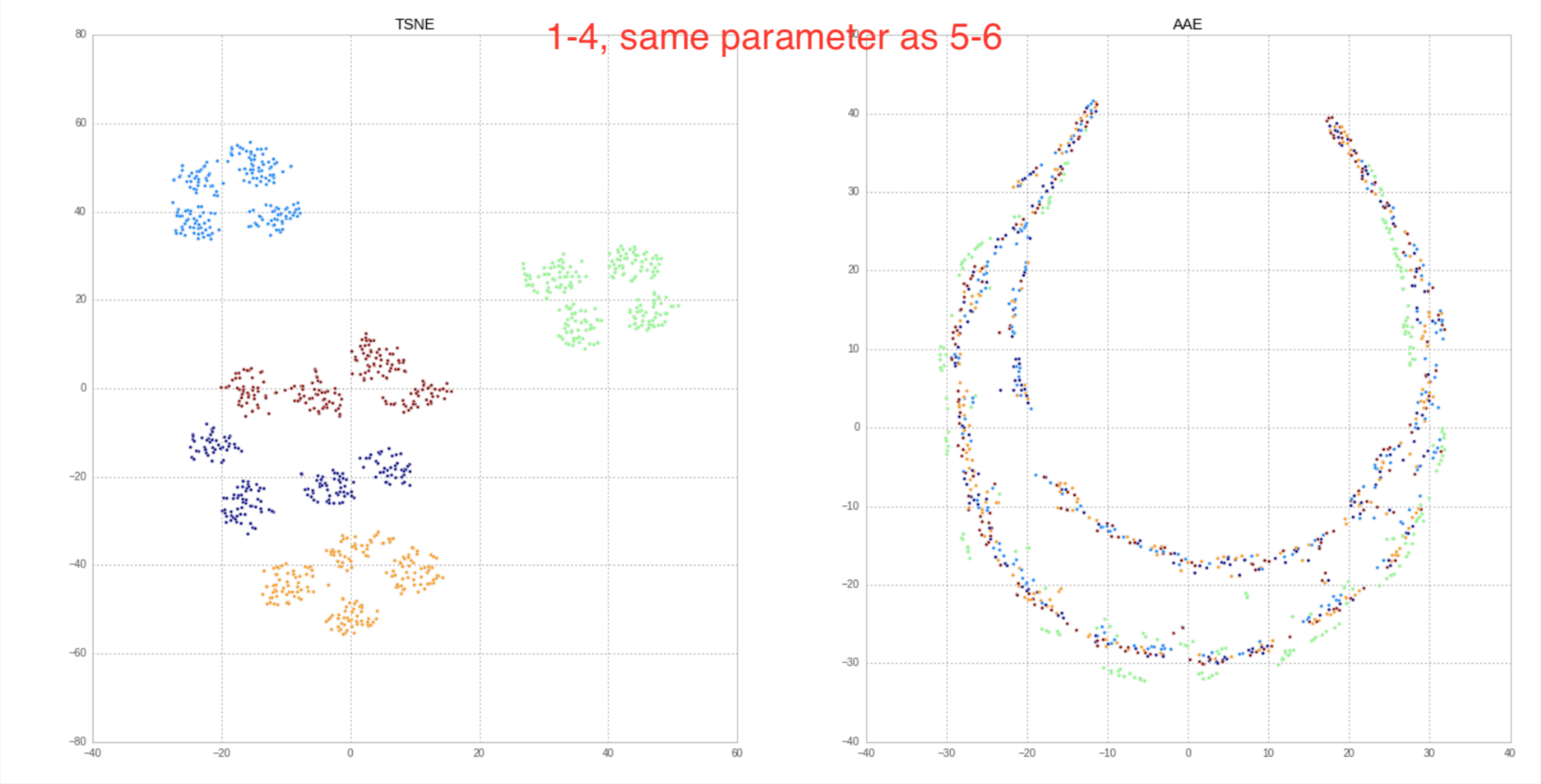
Experiments

Baseline: AAE + tSNE



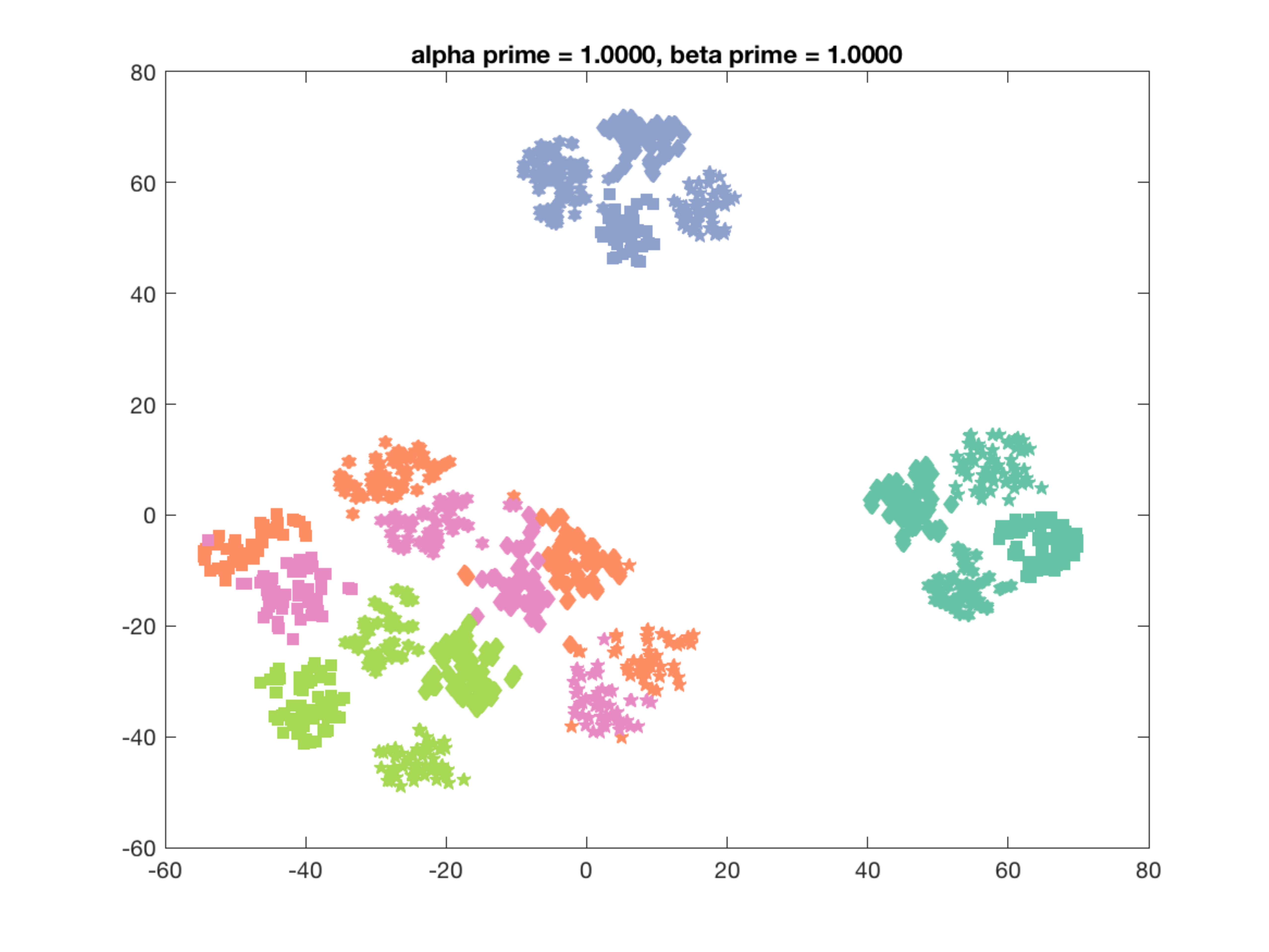
Experiments

Baseline: AAE + tSNE



Experiments

Parameter sensitivity GIF



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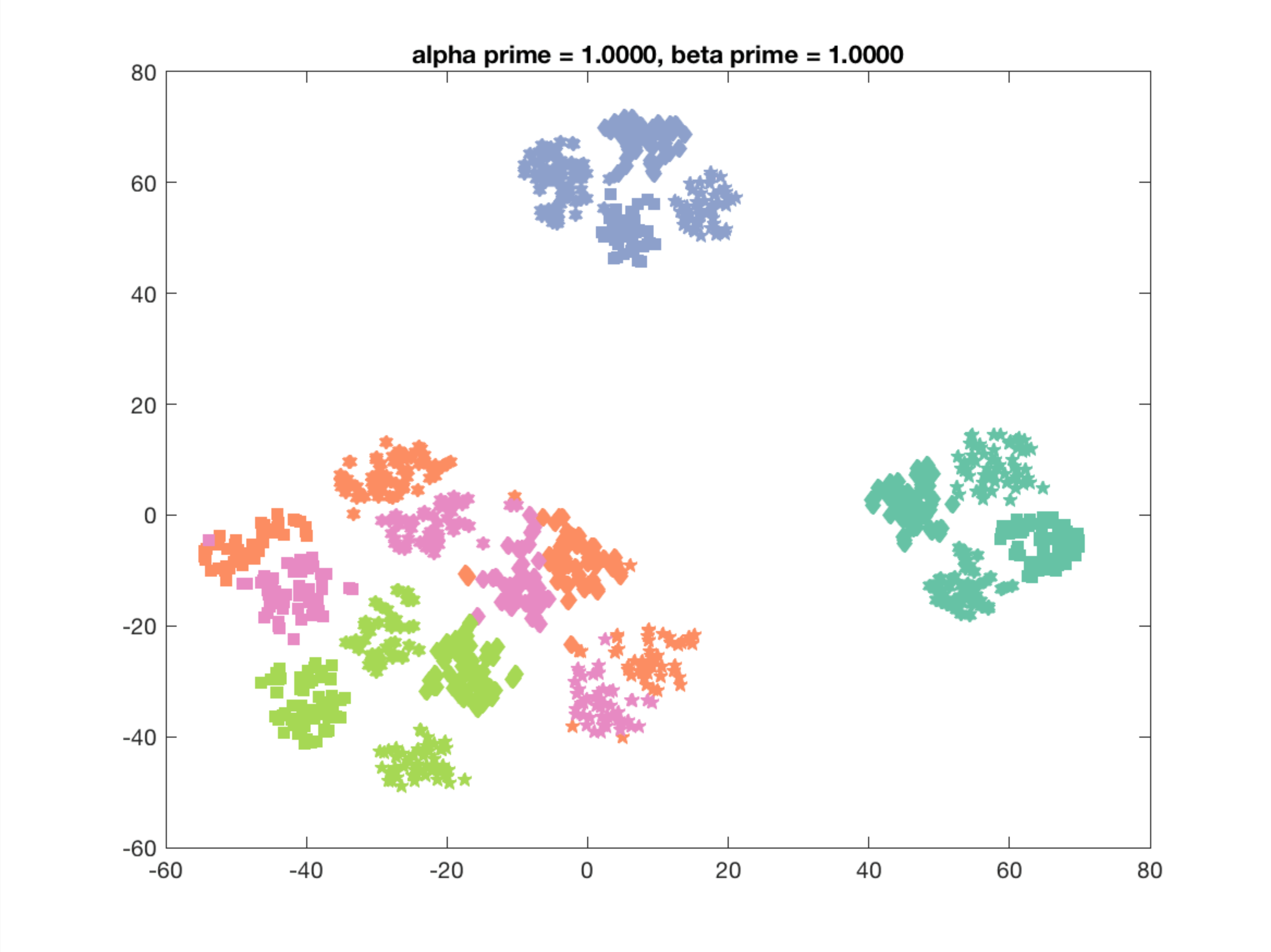

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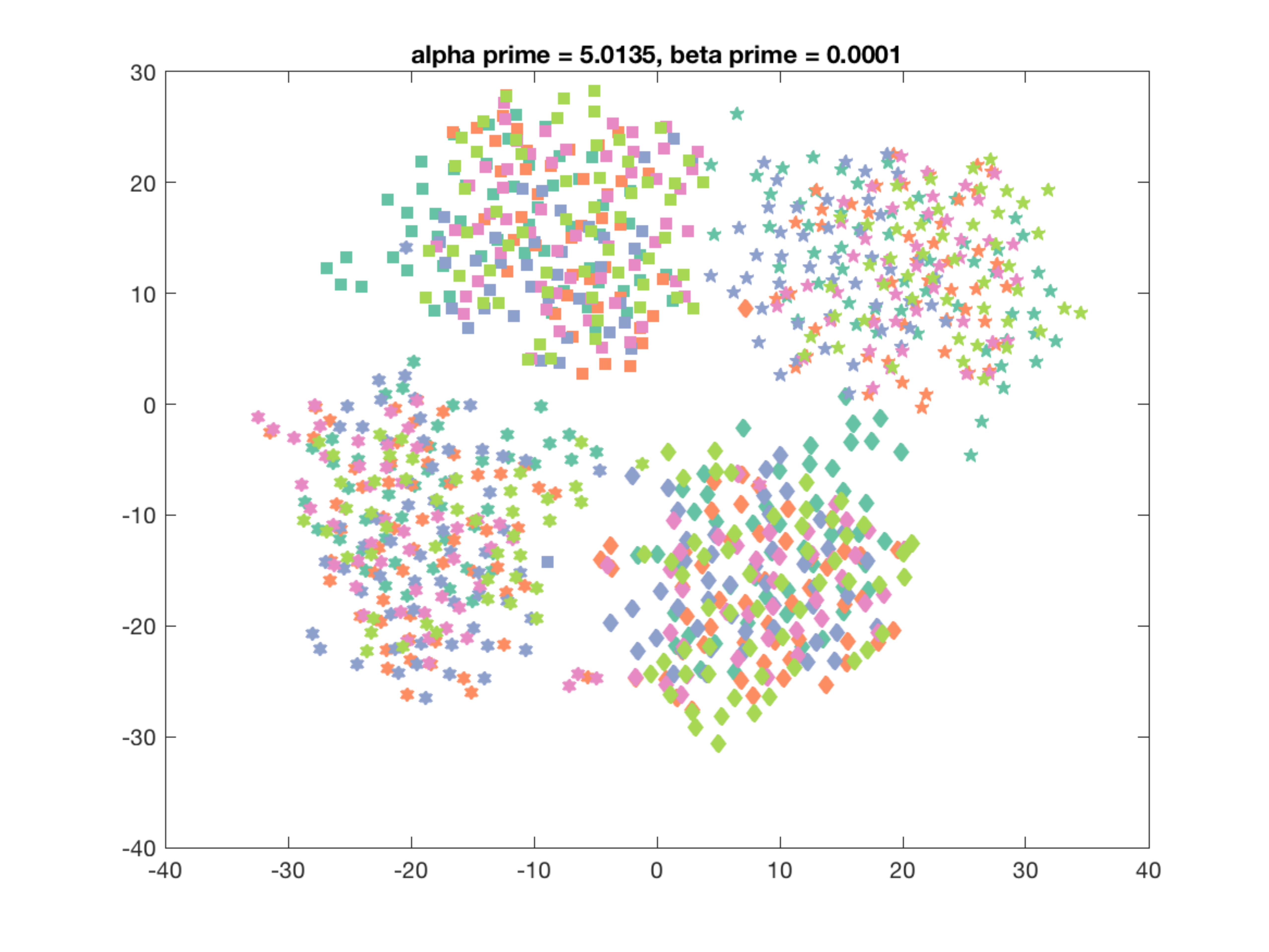
Parameter sensitivity GIF



Experiments

Runtime

- 100k x 128d data
- 55GiB RAM / 1GiB SWAP
- 24 x 2.494 GHz
- 9600s without approximation
- 9s per gradient update with tree approximation
- 52s per update with 500k x 128d data

Experiments

Interpretation methods

- Interpret cluster (in)consistent between tSNE and cTSNE
- Automatic cluster/region finding
- Histogram interpretation
- Logistic regression on sparse feature (e.g., links, tags)
- Random Forest on sparse feature
- Embedding space KNN
- Subgroup discovery based methods

Future Work

- Generalized framework
- Independence assumption
- Steerable / iterative data exploration: align or explain away
- Privacy preserving data analysis
- Optimization

Thanks