Enhancing Semi-Supervised Clustering: A Feature Projection Perspective

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Outline

$\Rightarrow$ Introduction

- The SCREEN Algorithm
- Experimental Results
- Related Works
- Conclusions

Introduction

- In many application domains:
  - ◇ Large volume of unlabeled data
  - ◇ Limited supervision:
    - * Labeled instances
    - * Pairwise instance constraints

- Semi-supervised clustering
  - ◇ Combining unlabeled and labeled instances
  - ◇ Improving the clustering performance through supervision

Research Motivation

- Various applications often contain high dimensional sparse data
  - text documents, market basket data

- Traditional semi-supervised clustering methods:
  - constraint-based, distance based, and hybrid methods

- Most existing methods are not designed for handling those data
  - Euclidean notion of density is not very meaningful in high-dimensional data

- There is a need to incorperate feature reduction into the process of semi-supervised clustering

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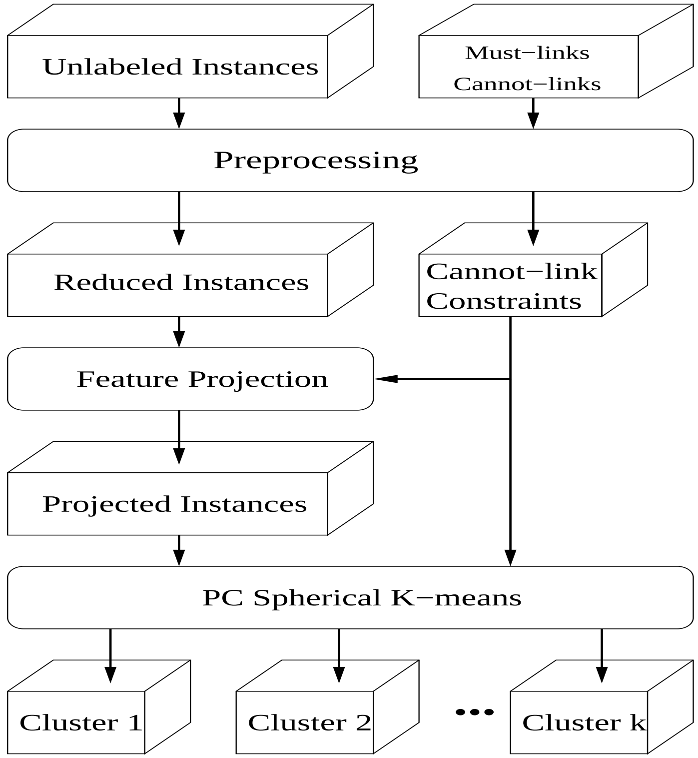
Problem Formulation

- Given:
  - A set of d-dimensional instances $\mathcal{X}$
  - A set of must-link constraints C_{ML}
  - A set of cannot-link constraints C_{CL}
  - A pre-specified reduced dimension $k \ll d$
  - A desired number of clusters K

- Find:
  - K clusters of instances represented in reduced k-dimensional vector which satisfies the given instance constraints.

The Framework of the SCREEN Algorithm



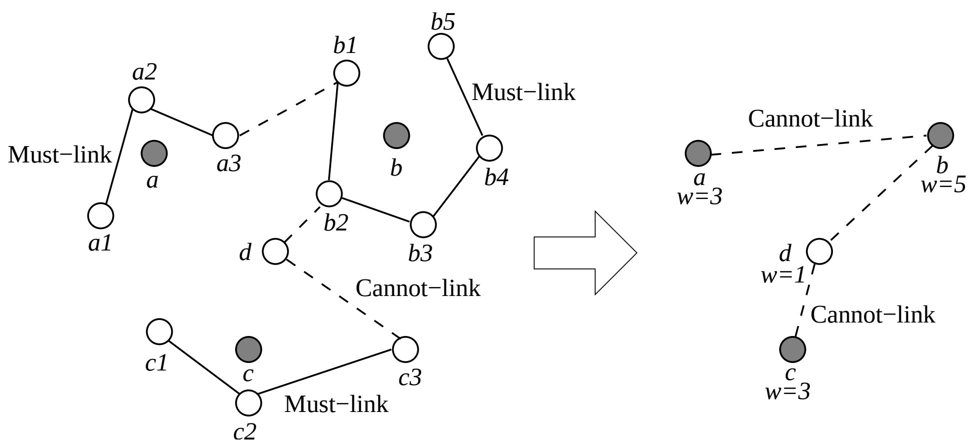
Step 1 Initialization

Step 2 Constraint-guided feature projection

Step 3 Constrained Spherical k-means on projected data

Initialization - An Example

- Since must-links represent an equivalence relation, it enables us to replace each transitive closure of must-links with its average.
- sets $\{a_1, a_2, a_3\}$, $\{b_1, b_2, b_3, b_4, b_5\}$, and $\{c_1, c_2, c_3\}$ represent different transitive closures enforced by must-links.



- After the initialization:
  - ◇ The pairwise constraints C_{ML} and C_{CL} are reduced to C'_{CL}
  - ◇ The original data sets $\mathcal{X}$ are reduced to $\mathcal{X}'$ with $\mathcal{W}'$

Constraint-Guided Feature Projection - SCREEN$_{PROJ}$

- Given
  - A set of cannot-link constraints C'_{CL}
  - A set of instances $\mathcal{X}'$ with weight $\mathcal{W}'$

- Objective: find an projection matrix F, such that

$$f = \sum_{(x'_1, x'_2) \in C'_{CL}} \|w_1 w_2 \cdot F^T (x'_1 - x'_2)\|^2$$

is maximized subject to the constraints

$$F_i^T F_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Solution To the Feature Projection Problem

- The Lagrangian of the above optimization problem is

$$L_{F_1,\ldots,F_k} = f(F_1, \ldots, F_k) - \sum_{l=1}^{k} \xi_l (F_l^T F_l - 1) \ .$$

which can be solved as

$$\begin{aligned} \frac{\partial L}{\partial F_l} &= 2MF_l - 2\xi_l F_l = 0 \qquad \forall l = 1, \ldots, k \\ \Rightarrow \ MF_l &= \xi_l F_l \qquad \forall l = 1, \ldots, k \ . \end{aligned} \tag{1}$$

Theorem 1 *Given the desired dimensionality* k $(k < d)$*, the set of* <u>*cannot-link*</u> *constraints* C'_{CL}*, and the covariance matrix* $M = cov(C)$*, the optimal projection matrix* $F_{d \times k}$ *is comprised of the first* k *eigenvectors of* M *corresponding to the* k *largest eigenvalues.*

Constrained Spherical K-means

- Updating rule in applying pairwise constraints
  - Given each cannot-link constraint $(x'_i, x'_j) \in C_{CL}$
  - Find two different cluster centroids $\mu_{x'_i}$ and $\mu_{x'_j}$ such that

$$w_i \cdot {x'}_i^T \mu_{x'_i} + w_j \cdot {x'}_j^T \mu_{x'_j}$$

    is maximized.
  - Assign x'_i and x'_j to these two centroids to avoid violating the constraints.

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Experimental Setup

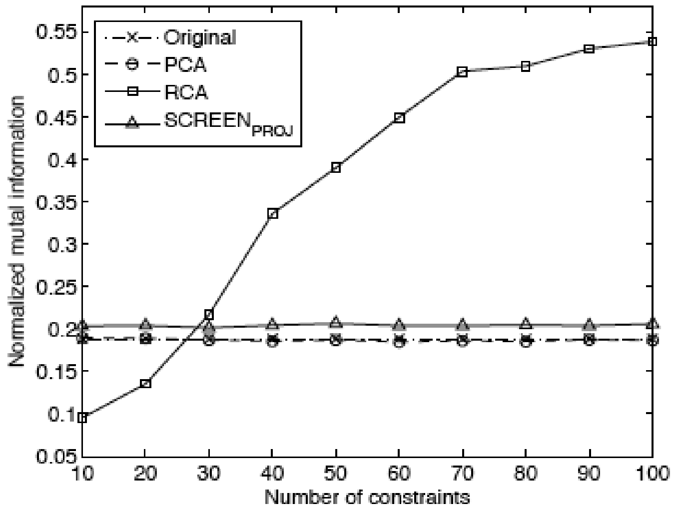
- Experimental Platform
  - GNU/Linux workstation with 4 Intel Xeon 2.8 GHz CPUs and 2G main memory
- Experimental Data Sets
  - Six data sets from UCI Machine Learning Repository
  - Six data sets from TREC collection
  - Nine data sets from 20-Newsgroups corpus
- Evaluation Measure: (Normalized Mutual Information)

$$NMI = \frac{I(\hat{Z}; Z)}{(H(\hat{Z}) + H(Z))/2}$$

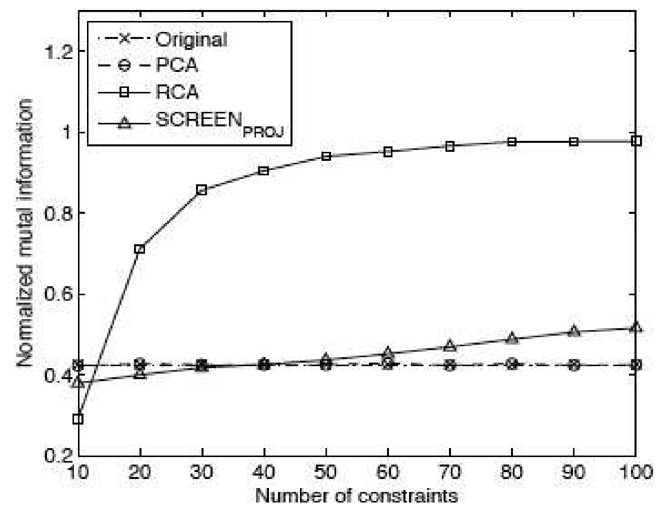
where $I(\hat{Z}; Z)$ is the mutual information between the random variables $\hat{Z}$ and Z, $H(Z)$ is the Shannon entropy of Z.

Effectiveness of SCREEN$_{PROJ}$ (1)

- Compared with original, PCA and RCA on low dimensional data
- Measured by NMI

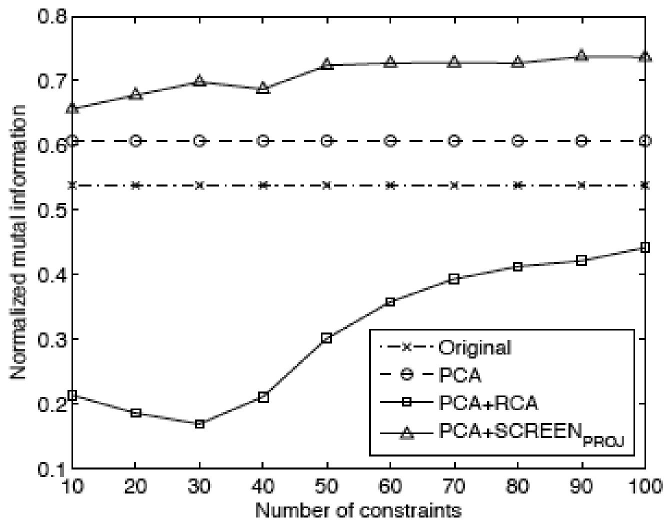


(e) Vehicle (N=846,C=4,D=18,d=5)

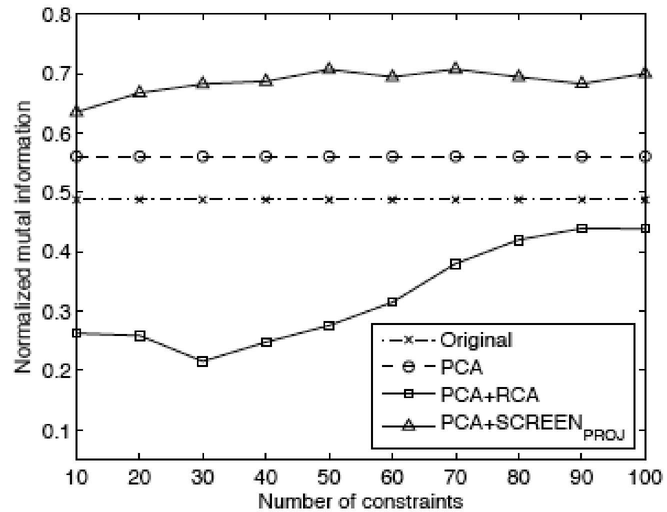


(f) Wine (N=178,C=3,D=13,d=5)

Effectiveness of SCREEN$_{PROJ}$ (2)



(a) tr11



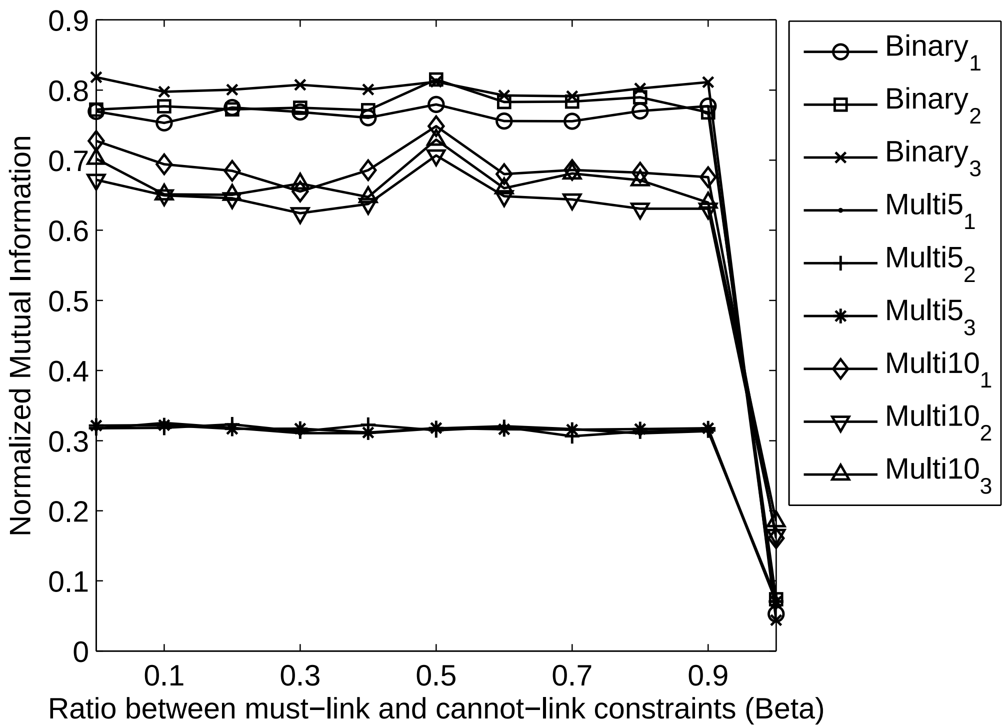
(b) tr12

- Conclusions:
  - ◇ RCA performs the best in the low dimensional data; however is not a good choice in handling high dimensional data
  - ◇ SCREEN$_{PROJ}$ is comparable to, or better than PCA in low dimensional data; especially archive good performance on high dimensional data

Must-links vs. Cannot-links

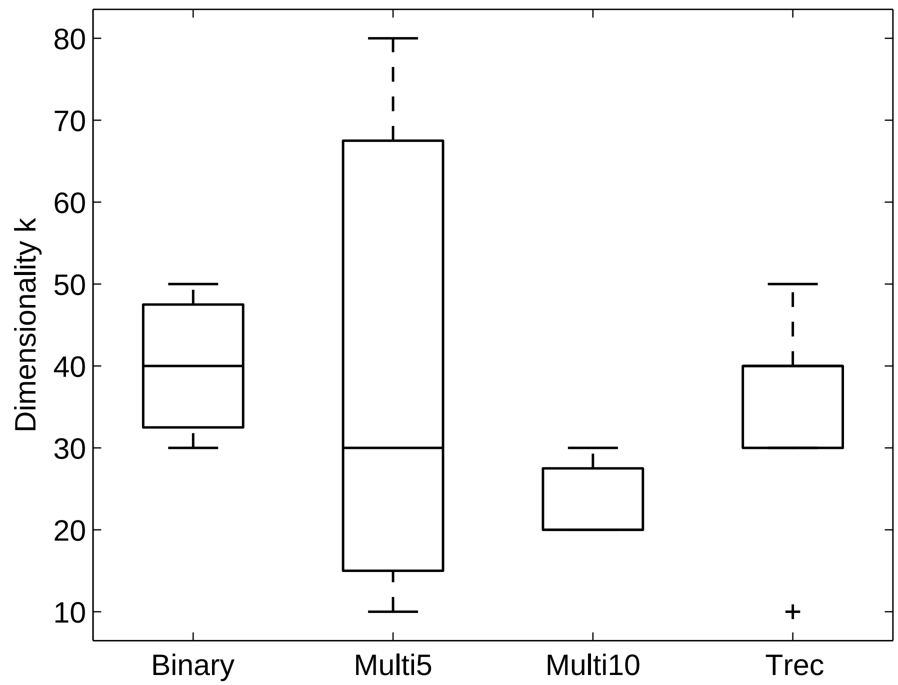
- Incorporate β into the previous objective function and varies from 0.0 to 1.0

$$f = (1-\beta)\cdot \sum_{(x_1,x_2)\in C_{CL}} \|F^T(x_1-x_2)\|^2 - \beta \cdot \sum_{(x_1,x_2)\in C_{ML}} \|F^T(x_1-x_2)\|^2$$



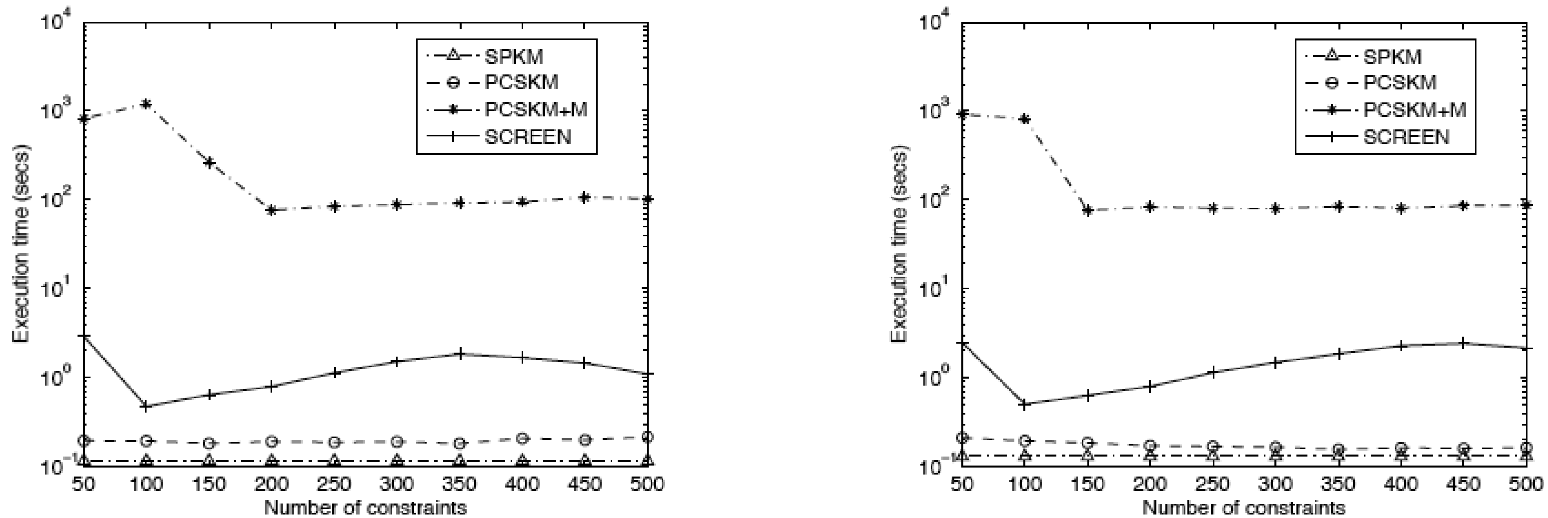
The Choice of Dimension K

- The SCREEN algorithm on different value of k from 10 to 100



- Clustering performance is maximized when k is between 20 and 40.

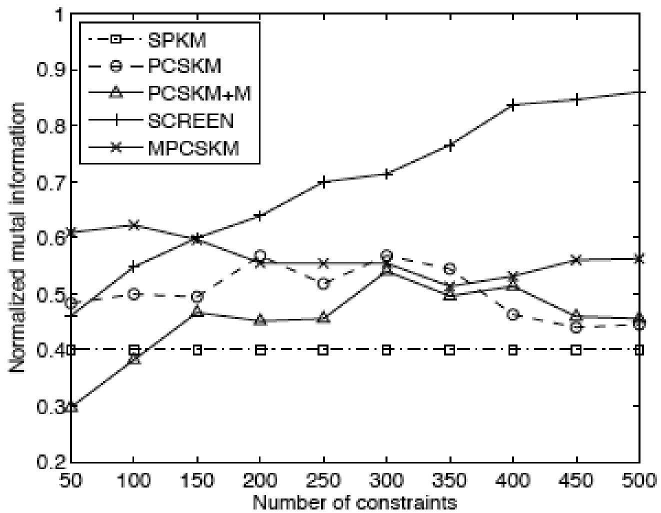
Computational Performance of the SCREEN Algorithm



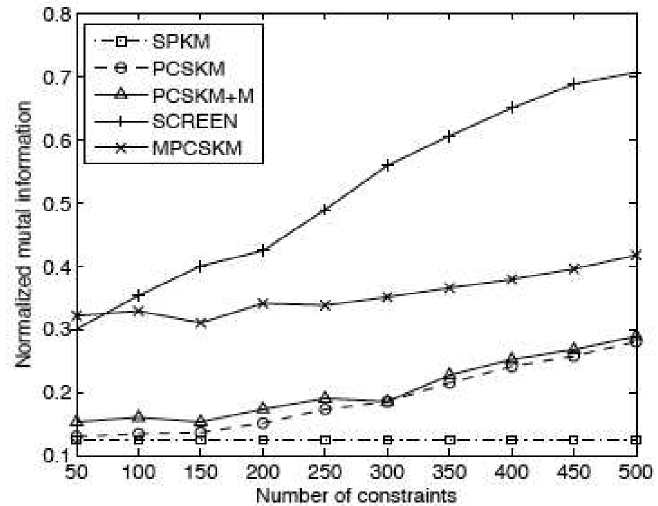
(b) $Multi5_1$ (c) $Multi10_1$

- SCREEN ranks third due the extra cost of feature projection.
- SCREEN is much faster than the PCSKM+M algorithm which employs metric learning in the high dimensional data.

Clustering Performance of the SCREEN Algorithm



(d) $Multi5_1$



(g) $Multi10_1$

- SCREEN is more stable compared to the other methods.
- SCREEN always outperforms the PCSKM+M via metric learning and MPCSKM via HMRF model.

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Related Works (1)

- From the perspective of semi-supervised clustering
  - ◇ Constraint-based methods (PCSKM)
    - guide the clustering process by supervision
  - ◇ Distance-based methods (PCSKM+M)
    - learn an adaptive distance based on constraints
  - ◇ Hybrid methods (MPCSKM)
    - combines them into an unified statistical framework

Related Works (2)

- From the perspective of feature projection
  - ◇ Principal Component Analysis (PCA)
    - without utilizing any supervision
  - ◇ Fisher's Linear Discriminant Analysis (LDA)
    - need to get the exact class information
  - ◇ Relevant Component Analysis (RCA)
    - based only on must-link constraints
  - ◇ Many others: projected clustering, CLIQUE

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Conclusions

- Formulate the constraint-guided feature projection into an optimization problem and give a closed-form solution
- Propose the SCREEN algorithm which integrates feature projection into semi-supervised clustering
- Experimental comparison between the SCREEN algorithm and the other methods

Questions?

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Thank You!