Software mention clustering using machine learning

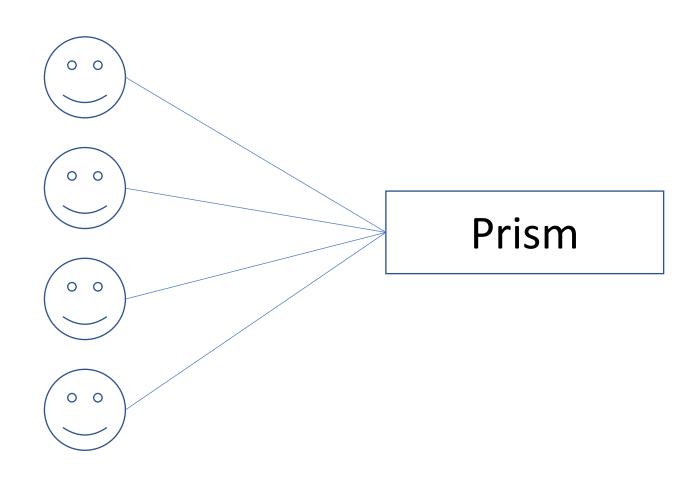
Daniel Garijo and Jinseok Kim

Mapping the Impact of Research Software in Science

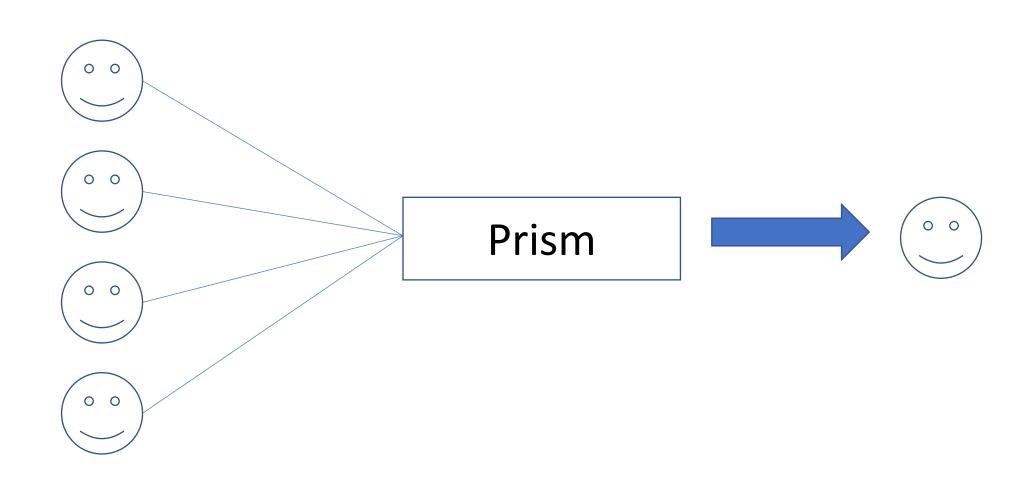
Chan Zuckerberg Initiative, Redwood City, California 24-27 October 2023

- Figures and tables presented in these slides are sourced directly from a paper currently under review:
- Jinseok Kim and Jenna Kim (Under Review). 'ANDez: An Open-Source Python Tool for Author Name Disambiguation Using Machine Learning'.

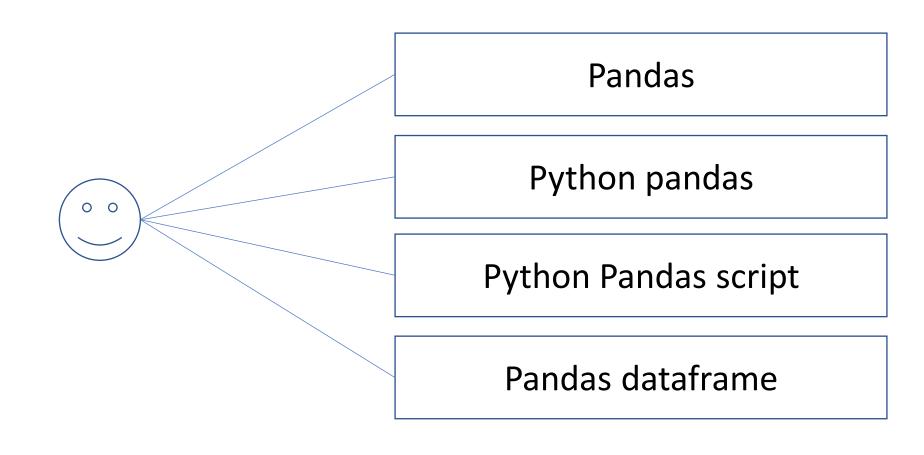
Software names are ambiguous: Homonyms



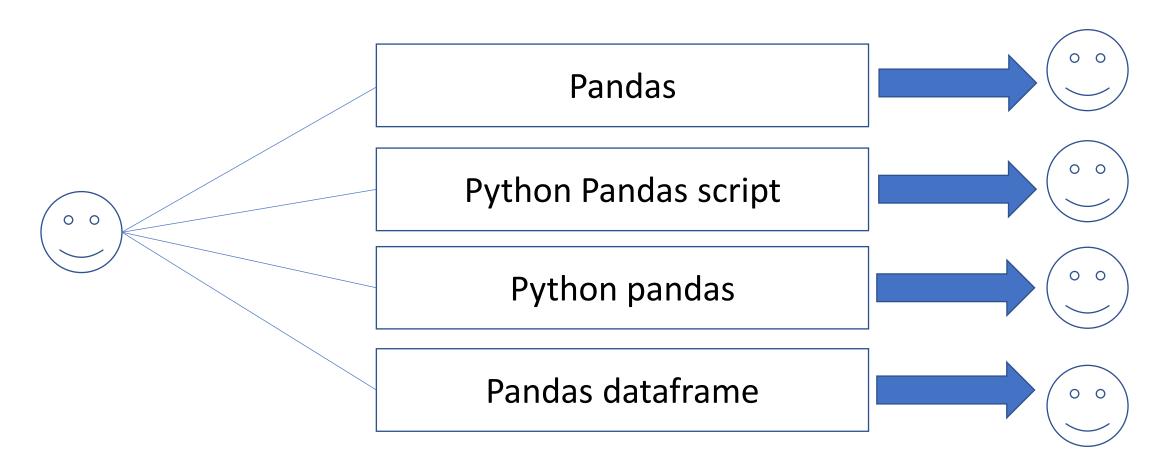
Why matters? Homonyms → Merging of software entities



Software names are ambiguous: Synonyms



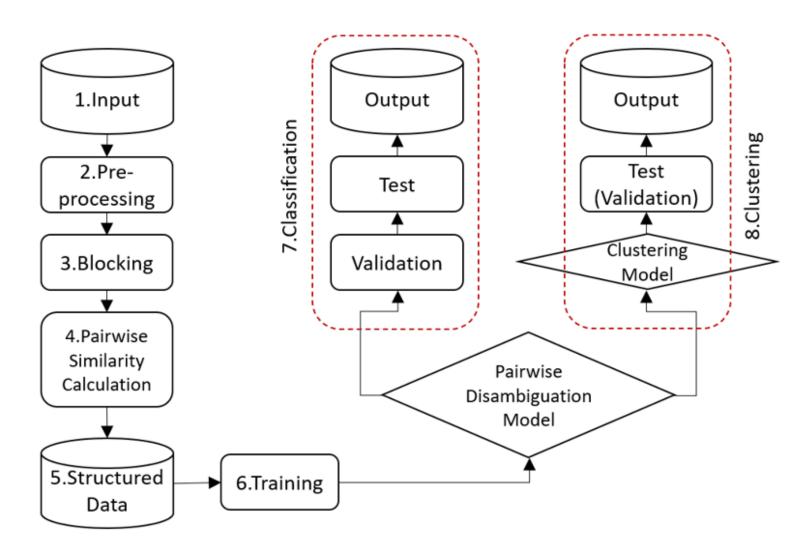
Why matters? Synonyms → Splitting of software entities



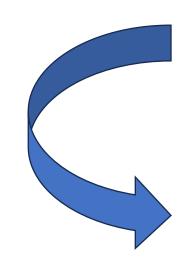
Using ANDez for software mention disambiguation

- An open-source platform that consolidates the processes of multiple high-performing ML techniques for classification and clustering in author name disambiguation (AND) → Modified for software name disambiguation (SND)
- Created using Python and widely used ML libraries (esp. scikit-learn)
- Offers a transparent and uniform framework for AND that brings together the execution of several ML methodologies
- GitHub repo: https://github.com/TEEDLab/ANDez
- Codeocean capsule: https://doi.org/10.24433/CO.0959364.v1

Workflow in ANDez



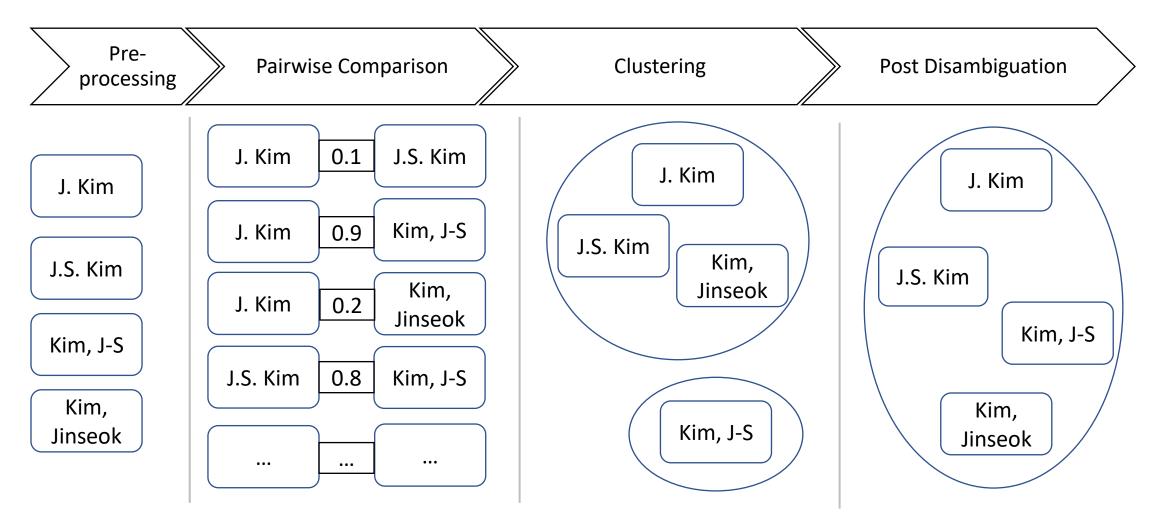
Key of name disambiguation in ANDez: Pairwise similarity comparison



	InstanceID	AuthorName	Affiliation	Coauthor	Journal	Title Tokens
1	1	Kim, Jinseok	Western Michigan Univ.	N. J. Reddy	Mechanics of Advanced Materials and Structures	Gradient, elasticity, plates,
-	2	Kim, Jinseok	Univ. of Michigan	N/A	JASIST	Publication, conference,
4	1	Kim, Jinseok	Western Michigan Univ.	N. J. Reddy	Mechanics of Advanced Materials and Structures	Gradient, elasticity, plates,
-	3	Kim, Jinseok	Univ. of Illinois	Jana Diesner	JASIST	Disambiguation, network,
2	3	Kim, Jinseok	Univ. of Illinois	Jana Diesner	JASIST	Disambiguation, network,
5	2	Kim, Jinseok	Univ. of Michigan	N/A	JASIST	Publication, conference,

PairID	InstanceID	AuthorName	Affiliation	Coauthor	Journal	Title	Label
1	1 2	1.0	0.4	0.0	0.0	0.2	0
2	1 3	1.0	0.4	0.2	0.0	0.1	0
3	2 3	1.0	0.5	0.0	1.0	0.4	1

Workflow of name dismbiguation



Requirements for ANDez implementation for software names

- Raw data should be converted into specific formats
 - **Signature file**: contains information specific to an instance like instance ids, record ids, position of mentions in bylines (not required for SND), name string, auxiliary information such as existence of version mention, and class labels for each instance
 - **Record file**: contains information specific to a record like record ids, record years, record venues (e.g., journal names), list of authors, sentences or paragraphs with software mentions, record keywords, and any other information to be used
 - Cluster file: contains information of cluster membership of an instance to be used for training and evaluation of machine learning models

Examples of input files formatted for ANDez using author name disambiguation cases

<u>Kim, Jinseok</u> and Reddy, J. N. (2017) Modeling of functionally graded smart plates with gradient elasticity effects. *Mechanics of Advanced Materials and Structures*

<u>Kim, Jinseok</u> (2019) Author-based analysis of conference versus journal publication in computer science. *JASIST*

<u>Kim, Jinseok</u> and Diesner, Jana (2016) Distortive effects of initial-based name disambiguation on measurements of large-scale coauthorship networks. *JASIST*

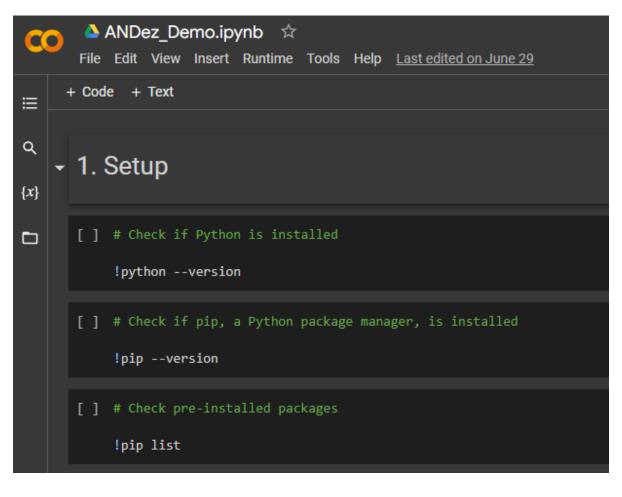
	Papers							
PaperID PubYear Journal			Authors	Title				
1	2017	Mechanics of Advanced Materials and Structures	Kim, Jinseok Reddy, J. N.	Modeling of functionally				
2	2019	JASIST	Kim, Jinseok	Author-based analysis				
3	2016	JASIST	Kim, Jinseok Diesner, Jana	Distortive effects of				

Instances							
InstanceID	PaperID	Position	AuthorName	Affiliation			
1	1	1	Kim, Jinseok	Western Michigan Univ.			
2	2	1	Kim, Jinseok	Univ. of Michigan			
3	3	1	Kim, Jinseok	Univ. of Illinois			

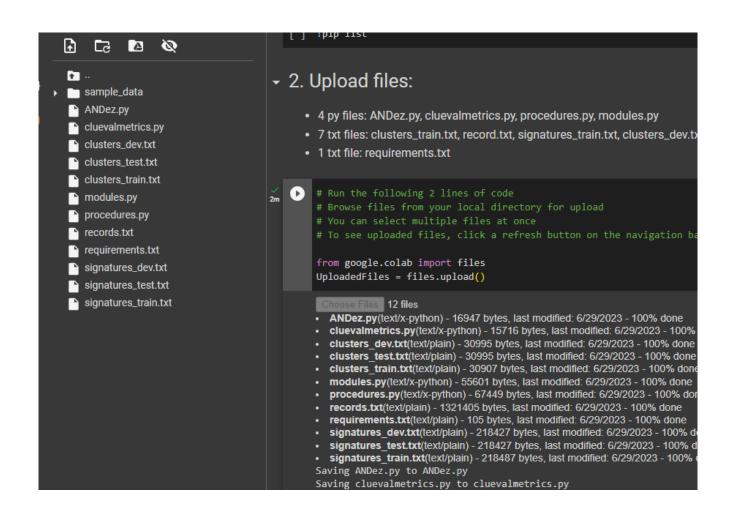
Clusters			
ClusterID	MemberInstanceID		
1	1		
2	2 3		

Demo: Setup using Google Colab

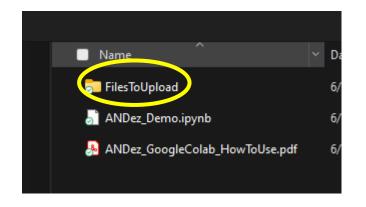
NOTE: This demonstration utilizes author name disambiguation files as an example. Once the software name files are formatted appropriately, the same implementation process outlined here will be applied for AND.

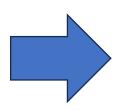


Upload Files



Upload all the files downloaded





Name	Date mod
₹ ANDez.py	6/29/2023
👼 cluevalmetrics.py	6/29/2023
♂ clusters_dev.txt	6/29/2023
♂ clusters_test.txt	6/29/2023
♂ clusters_train.txt	6/29/2023
👼 modules.py	6/29/2023
👼 procedures.py	6/29/2023
♂ records.txt	6/29/2023
📝 requirements.txt	6/29/2023
♂ signatures_dev.txt	6/29/2023
♂ signatures_test.txt	6/29/2023
♂ signatures_train.txt	6/29/2023

Install extra packages on a local machine, more packages might need to be installed

```
2. Upload files:
     • 4 py files: ANDez.py, cluevalmetrics.py, procedures.py, modules.py

    7 txt files: clusters_train.txt, record.txt, signatures_train.txt, clusters_dev.txt, signature

     · 1 txt file: requirements.txt
       # Run the following 2 lines of code
        # Browse files from your local directory for upload
        # You can select multiple files at once
        # To see uploaded files, click a refresh button on the navigation bar at the
        from google.colab import files
        UploadedFiles = files.upload()
  [ ] # Install python packages
        !pip install -r requirements.txt
       Collecting unidecode==1.3.6 (from -r requirements.txt (line 1))
         Downloading Unitecode-1.3.6-py3-none-any.whl (235 kB)
                                                     - 235.9/235.9 kB 9.4 MB/s eta 0:00
       Collecting jellyfish==0.11.0 (from -r requirements.txt (line 2))
         Downloading jellyfish-0.11.0-cp310-cp310-manylinux 2 17 x86 64.manylinux2014
```

Before you run main file (ANDez.py), make sure that ...

```
3. Run main file: ANDez.py
     # ANDez is an open-source framework that integrates the workflows of several high-performing machine learning methods
     # for classification and clustering in author name disambiguation.
     # ANDez was developed under a grant from the National Science Foundation
     # (NSF NCSES Award # 1917663: Creating a Data Quality Control Framework for Producing New Personnel-Based S&E Indicators
     # and its supplementary fund program, Research Experiences for Undergraduates (REU).
     # Author:
     # 1. Jinseok Kim (Ph.D.): Institute for Social Research and School of Information, University of Michian Ann Arbor
     # 2. Jenna Kim: School of Information Sciences, University of Illinois at Urbana-Champaign
     .______,
     # NOTE: Run this script with 'procedures.py', 'modules.py', 'cluevalmetrics.py'
           after placing all the files in the same directory
     _____
     import time
     import uuid
     from datetime import timedelta
     from procedures import *
```

Set parameters (= options): The first choice you need to make...

```
For details on parameter choices during disambiguation, see a paper below
(1) Kim, J., & Kim, J. (2020). Effect of forename string on author name disambiguation.
   Journal of the Association for Information Science and Technology, 71(7), 839-855
(2) Kim, J., Kim, J., & Owen-Smith, J. (2019). Generating automatically labeled data for
   author name disambiguation: an iterative clustering method. Scientometrics, 118(1), 253-280.
(3) Kim, J., & Owen-Smith, J. (2020). Model Reuse in Machine Learning for Author Name Disambiguation:
   An Exploration of Transfer Learning. IEEE Access, 8, 188378-188389. doi:10.1109/ACCESS.2020.3031112
### Select model training or application ###
Two options:
(1) train and save a model: "train"
(2) test the trained model: "test"
model usage = "test"
```

Set parameters (= options): The first choice you need to make...

```
For details on parameter choices during disambiguation, see a paper below
(1) Kim, J., & Kim, J. (2020). Effect of forename string on author name disambiguation.
   Journal of the Association for Information Science and Technology, 71(7), 839-855
(2) Kim, J., Kim, J., & Owen-Smith, J. (2019). Generating automatically labeled data for
    author name disambiguation: an iterative clustering method. Scientometrics, 118(1), 25
(3) Kim, J., & Owen-Smith, J. (2020). Model Reuse in Machine Learning for Author Name Disa
    An Exploration of Transfer Learning. IEEE Access, 8, 188378-188389. doi:10.1109/ACCESS
### Select model training or application ###
Two options:
(1) train and save a model: "train"
(2) test the trained model: "test"
model usage
```

Type input file names

```
######## Parameters for training & development #########
If you want to train and save a model,
you can change values of the follwing parameters
before you run the main code
### 1-1. Type in file names ###
Input files are required to be prepared in a specific format
(1) signature file: instance id, paper id, author byline position, name string, affiliation, etc.
(2) record file: paper id, publication year, venue name, author list, title, etc.
              > Author names in the author list are seperated by vertical bar
(3) cluster file: cluster id and instance id list
             > Instance ids in instance id list are separated by vertical bar
Each file is created in .txt and columns are separated by tab.
Please see the example files provided with this code set.
train instance file = "signatures train.txt"
train cluster file = "clusters train.txt"
train record file = "records.txt"
dev instance file = "signatures dev.txt"
dev cluster file = "clusters dev.txt"
dev_record_file = "records.txt"
```

Input file format

Kim, Jinseok and Reddy, J. N. (2017) Modeling of functionally graded smart plates with gradient elasticity effects. *Mechanics of Advanced Materials and Structures*

<u>Kim, Jinseok</u> (2019) Author-based analysis of conference versus journal publication in computer science. *JASIST*

Kim, Jinseok and Diesner, Jana (2016) Distortive effects of initial-based name disambiguation on measurements of large-scale coauthorship networks. *JASIST*

	Papers							
PaperID PubYear		PubYear	Journal	Authors	Title			
•	1	2017	Mechanics of Advanced Materials and Structures	Kim, Jinseok Reddy, J. N.	Modeling of functionally			
	2	2019	JASIST	Kim, Jinseok	Author-based analysis			
	3	2016	JASIST	Kim, Jinseok Diesner, Jana	Distortive effects of			

Instances						
InstanceID	PaperID	Position	AuthorName	Affiliation		
1	1	1	Kim, Jinseok	Western Michigan Univ.		
2	2	1	Kim, Jinseok	Univ. of Michigan		
3	3	1	Kim, Jinseok	Univ. of Illinois		

	Clusters		
ClusterID	MemberInstanceID		
1	1		
2	2 3		

Blocking

```
### 1-2. Choose a blocking method ###
Blocking is a step to collate name instances to be compared with each other
The blocking method selected here is applied to both training and test data
Three options are available
(1) first initial: name instances that have the same surname and first forename initial are compared
       e.g., 'kim, jinseok' vs 'kim, j' > They share 'kim, j'
(2) full name: name instances that have the same string are compared
       e.g., 'kim, jinseok' vs 'kim, jinseok' > They share 'kim, jinseok'
(3) forename strip: name instances that have the same surname and n characters of forename are compared
       e.g., 'kim, jinseok' vs 'kim, jin s' > They share 'kim, jin' (if n == 3)
For more details on blocking and 3 options, see the paper below
    Kim, J., & Kim, J. (2020). Effect of forename string on author name disambiguation.
       Journal of the Association for Information Science and Technology, 71(7), 839-855. doi:10.1002/asi.24298
blocking_method = "first_initial"
```

Similarity calculation metric

```
### 1-3. Choose a similarity calculation metric ###

"""

(1) cos: cosine similarity
(2) jac: Jaccard similarity
(3) jrw: Jaro-Winkler similarity

"""

similarity_metric = "cos"
```

Machine learning algorithms

```
### 1-4. Choose a classifier for pairwise similarity comparison ###
(1) GB: Gradient Boosting
(2) RF: Random Forests
(3) LR: Logistic Regression
(4) NB: Naive Bays;
(5) SVM: Support Vector Machine
(6) DT: Decision Tree;
Choice of multiple classifier names available: e.g., classifier lists = ['LR', 'RF', 'SVM']
URLs for details on each clssifier are available in procedures.py
                                                                        ··''' select classifiers '''
                                                                         if classifier name == "RF":
classifier_name_list = ['RF']
                                                                          ··''' · Random · Forest · ''' ·
                                                                         .....#.URL.->..https://scikit-learn.org/stable/modules
                                                                              classifier = RandomForestClassifier(
                                                                                               \cdots \cdots n estimators = \cdot 500,
                                                                                      \cdots  jobs \cdots = 8,
                                                                                                 ·····random state = 1,
                                                                                            ·····verbose····=·0
                                                                         elif classifier name == "GB":
                                                                        ·····Boosting·'''
```

·····#·URL·->··https://scikit-learn.org/stable/modules

·····max depth····=·9,

 $\cdots \cdots n$ estimators $\sim = \cdot 500$,

·····classifier = GradientBoostingClassifier(

10-fold cross validation

```
### 1-5. 10-fold cross validation is performed? ###

"""

(1) 1: yes
(2) 0: no

"""

cross_validation = 1
```

Producing classification results

Choosing clustering algorithms

```
### 1-7. Choose a clustering algorithm ###
Clustering is a process of an algorithm to collate name instances into clusters
(1) hier: hierarchical agglomerative clustering
       -> NOTE! you must change below options < clusterer blocking on = 1, cluster count = None >
       -> This process is implemented by the BEARD library for computational efficiency as introduced in
          Louppe, G., Al-Natsheh, H. T., Susik, M., & Maguire, E. J. (2016).
          Ethnicity Sensitive Author Disambiguation Using Semi-supervised Learning.
          Knowledge Engineering and Semantic Web, Kesw 2016, 649, 272-287.
(2) db: DBSCAN
(3) spectral: spectral
(4) kmeans: K-Means
(5) agg: agglomerative clustering: change below options <clusterer blocking on = 0, cluster count = integer number>
URLs for details on each clssifier are available in modules.py
clustering algorithm = "hier"
cluster blocking on = 1 # 1 for clustering with blocking applied (hierarchical); 0 for other clustering methods
cluster count = None # "None" for hierarchical clustering; integer(e.g., 1000) for DBSCAN, spectral, KMeans or agglomerative
```

A special parameter for 'hier' (Hierarchical Agglomerative Clustering – HAC- algorithm)

```
### 1-8. If 'hier' is chosen, what is a threshold value? ###

"""

Set a threshold value to filter instance pairs to be put into the same cluster
between 0 and 1
A threshold value is a distance, i.e., 1 - similarity score, between name instances.
E.g., A threshold value of 0.3 is roughly equal to 70 % of probability of name instances
    referring to the same author entity
The lower the threshold value is, the higher the precision score is.

"""

threshold_list = [0.1, 0.3, 6]  # [0] if clustering algorithms other than 'hier' are used

# <- if various thresholds need to be used, put a starting threshold, an end
# e.g., [0.1, 0.3, 5]: this generates a list of thresholds [0.1, 0.15, 0.2, 0.25, 0.3]</pre>
```

Choosing evaluation metrics

```
### 1-9. Which clustering evaluation metric do you want to use? ###
.....
(1) cluster-f: cluster-f precision/recall/f1
(2) k-metric: k-metric precision/recall/f1
(3) split-lump: splitting & lumping error precision/recall/f1
(4) pairwise-f: paired precision/recall/f1
(5) b-cubed: b3 precision/recall/f1
For more details on clustering evaluation metrics, see a paper below
Kim, J. (2019). A fast and integrative algorithm for clustering performance evaluation
    in author name disambiguation. Scientometrics, 120(2), 661-681.
*******
clustering metric = "b-cubed"
```

Output with or without IDs

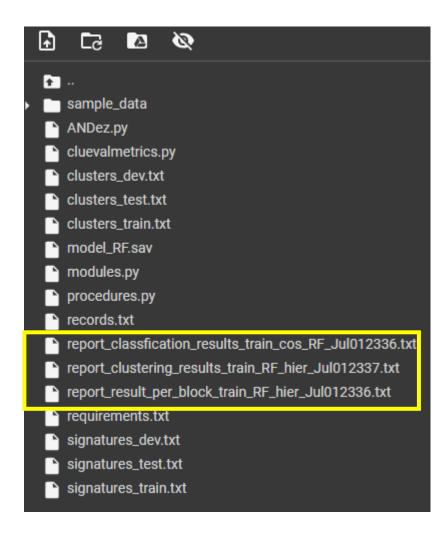
```
### 1-10. Would you like to assign a distinct identifier to each cluster? ###
enable cluster id = True
enable cluster id = False
The parameter enable cluster id controls whether a unique identifier is
assigned to each cluster within the namespace "550e8400-e29b-41d4-a716-44665544abcd".
This can be useful for tracking individual clusters throughout an analysis.
To enable cluster ID, set enable cluster id to True. The output file includes
IDs in the first column and cluster lists in the second column with a tab as a delimiter.
To disable cluster ID, set enable cluster id to False.
The namespace used in this script is a UUID (Universally Unique Identifier)
generated with the value '550e8400-e29b-41d4-a716-44665544abcd'. A UUID is a 128-bit
identifier that is globally unique and can be used to prevent naming conflicts
between different systems or entities. This namespace is used to create deterministic
UUIDs using the uuid5() function from the uuid module, which takes a namespace and
a name as input and generates a UUID based on them.
enable cluster id = True
cluster_id_namespace = uuid.UUID('550e8400-e29b-41d4-a716-44665544abcd')
```

Progress report

```
Instance pairs created...
Count of Pairs
    all|positive|negative : 97335|17051|80284
Ratio sampling NOT conducted...
Blocking method: 'first_initial' is selected
.... Instance pairs for training created
Similarity calculation metric: 'cos' is selected
10-fold cross validation is being conducted...
Round-1: Precision|Recall|F1|Support
-class0: 0.7180|0.5657|0.6328|1706
-class1: 0.9117|0.9528|0.9318|8028
-RMSE: 0.3392
-Confusion Matrix:
[[ 965 741]
 [ 379 7649]]
Round-2: Precision | Recall | F1 | Support
```

Evaluation report for classification and output files

Cl	====== Classification Report ======						
Confusion Mat	rix:						
	[[8875 7855] [3917 73949]]						
Evaluation Sc	ore:						
	precision	recall	f1-score	support			
class 0	0.69	0.53	0.60	16730			
class 1	0.90	0.95	0.93	77866			
accuracy			0.88	94596			
macro avg	0.80	0.74	0.76	94596			
weighted avg	0.87	0.88	0.87	94596			
File Created:	'report_cla	ssficatio	n_results_t	train_cos_RF	:_Jul012025.txt'		



Report for classification results

```
report classification results train cos RF Jul012336.txt X
  1 pair id|inst id 1|inst id 2|author|coauthor|title|venue|class prob|predicted class|true class
  2 1 | 100203015 | 100742353 | 1.0 | 0.1826 | 0.1064 | 0.0157 | 0.65 | 1 | 0
  3 2 100203015 104289887 0.9608 0.0463 0.1308 0.0177 1.0 1 0
  4 3 | 100203015 | 116701245 | 1.0 | 0.0 | 0.3029 | 0.0 | 0.328 | 0 | 0
  5 4 | 100203015 | 45167785 | 1.0 | 0.0 | 0.4293 | 0.0 | 0.002 | 0 | 0
  6 5 | 100203015 | 52190776 | 1.0 | 0.0 | 0.2209 | 0.0 | 0.392 | 0 | 0
  7 6 | 100203015 | 52536645 | 1.0 | 0.0891 | 0.1391 | 0.0081 | 0.676 | 1 | 0
  8 7 | 100203015 | 63741921 | 1.0 | 0.0255 | 0.1687 | 0.0092 | 0.846 | 1 | 0
  9 8 | 100203015 | 71573850 | 0.9608 | 0.0563 | 0.1655 | 0.0081 | 0.994 | 1 | 0
 10 9 | 100203015 | 74992893 | 1.0 | 0.0255 | 0.142 | 0.0 | 0.97 | 1 | 0
 11 10 100203015 79959401 1.0 0.4678 0.5259 1.0 0.0 0 0
 12 11 | 100203015 | 93888600 | 1.0 | 0.0 | 0.1958 | 0.0 | 0.176 | 0 | 0
 13 12 100203015 97210151 1.0 1.0 0.5509 0.0087 0.0 0 0
 14 13 | 100315950 | 62359481 | 1.0 | 0.094 | 0.1772 | 0.1234 | 0.798 | 1 | 0
 15 14 | 100315950 | 64590004 | 1.0 | 0.0 | 0.2606 | 0.4088 | 0.06 | 0 | 0
 16 15 | 100315950 | 70289768 | 1.0 | 0.2881 | 0.385 | 0.5547 | 0.01 | 0 | 0
 17 16 100315950 71273117 1.0 0.2921 0.1714 0.036 0.82 1 0
```

Report for clustering results

```
report clustering results train RF hier Jul012337.txt X
 1 49db20bb-a065-55e5-982c-c36d54ddf5ae
                                          64312446
 2 37d9d320-797b-5c6b-b6f8-ea45ebbb0335
                                           72185358 72642743
                                          92914603 | 93400261 | 95988534 | 100812740 | 10287 | 1880 | 104577273 | 1083
 3 6a48c0c1-df5e-5e86-85b2-f527a1bf4196
                                          61321893 | 62522259 | 101178554
 4 52227767-ada1-5375-844e-dc35e0a4e12b
                                           46207935 | 72619626 | 104289121 | 108923124
 5 87375728-912b-516f-b9a5-31326748ac80
 6 b32cc771-35b0-5ddf-a1ba-83a66fd34648
                                          52677682
 7 20b5037a-4d41-5d95-ad79-f5214f94c247
                                          116677551
 8 9b445386-363c-5d6b-9892-7037ac4189a4
                                          56946874
 9 7744a028-9b94-5286-b173-2405a5c71957
                                           79690488
10 c2473f6b-4257-5d39-973f-f91ce4e42411
                                           79890521
11 9ce01245-9656-5c91-8c5c-e037ebf6d0a9
                                          84863941 97799407
                                           51597905 | 57409174 | 90363736 | 102833104 | 10999 6549 | 116691770
12 304e04b4-bb91-5974-ba2d-ed34cd88b8ec
13 2020f429-ead3-5521-8046-37e288656c18
                                           34486842 | 48457754 | 56654678 | 59726189 | 61383783 | 66233904 | 747798
14 64e8d630-91cb-51b7-a5ee-0ec23c5ba225
                                           54034494 | 66676828
15 9a07e483-9070-5e26-8bbf-b465aaf0e454
                                           50914477
16 8f94ff0c-633b-5b5d-8610-137cc3be4082
                                           48261049 70845532
17 c888cb22-7734-5618-952c-507581b5777d
                                           61390968 72788896
18 c6338ea6-53a2-5c5e-963b-b7dc42e5bbf6
                                          48285552
19 434fb8f2-bef3-57f2-8058-429926ef4567
                                           36528978
20 8f122ccd-eb32-5331-b01c-ad4db803f8f2 33103606
```

Questions & Feedbacks

Jinseok Kim (jinseokk@umich.edu)