Constrains_Kmeans

September 25, 2017

0.0.1 This file contains Constraint-Kmeans alg. and relaed test results.

0.0.2 Contents

- I. n/a
- II. Helper functions
- III. Main function
- IV. Test & plots

```
In [194]: import pandas as pd
          import numpy as np
          import os
          from collections import Counter
          import matplotlib.pyplot as plt
          import pickle
          import time
          from pulp import *
          import random as rd
          import math
          import random as rd
          import sklearn.metrics as metrics
```

0.1 II. Helper functions

```
In [146]: # find cenriod for empty clusters:
          def furthest_centroids(j,k,lable,features):
              centroids = get_centroids(features, lable, j)
              for index in range(j,k):
                  temp = -1
                  furthest = 0
                  for i in range(len(features)):
                      if lable[i] is None:
                          dis = sum([euclidean_d(features[i],x) for x in centroids]
                          if dis>temp:
                              temp = dis
                              furthest = i
                  lable[furthest] = index
```

```
            centroids.append(features[index])
            #print(furthest)
        return centroids,lable

    # return the lable of a cluster that is most similar to the unassigned gr
    def fit_lable(group,features,lable,ub,k):
        temp = 1000000
        lable_of_closest = 0
        for i in range(k):
            seeds = [x for x in range(len(lable)) if lable[x] == i]
            if len(seeds) + len(group)>ub: continue
            dis = group_d(seeds, group,features)
            if  dis < temp:
                temp = dis
                lable_of_closest = i
        return lable_of_closest

    # return group distance
    def group_d(g1,g2,features):
        d = 0
        for i in g1:
            for j in g2:
                d += euclidean_d(features[i],features[j])
        return d

    # return object distance
    def euclidean_d(a,b):
        return math.sqrt(sum([(x-y)*(x-y) for (x,y) in zip(a,b)]))

    # get centriod
    def get_centroids(features, lable, k):
        centroids = []
        for i in range(k):
            seeds = [x for x in range(len(lable)) if lable[x] == i]
            centroids.append(np.mean(np.array([features[x] for x in seeds]),
        return centroids

    # end condition
    def shouldStop(oldCentroids, centroids, iterations, alpha, MAX_ITERATIONS
        if oldCentroids is None: return False
        if iterations > MAX_ITERATIONS: return True
        if sum([euclidean_d(x,y)>alpha for (x,y) in zip(oldCentroids,centroid
        return False

    # update lable
    def get_lable(features, lable, centroids, free, ub, k):
        for i in free:
            if lable[i] is not None and sum([1 for x in lable if lable[i]==x]
```

```
            temp = 1000000000
            lable_of_closest = lable[i]
            for j in range(k):
                if len([x for x in lable if x == j])<ub:
                    dis = euclidean_d(centroids[j],features[i])
                    if dis<temp:
                        temp = dis
                        lable_of_closest = j
            lable[i] = lable_of_closest
            #print(lable)
        return lable
```

0.2 III. Main function

```
In [246]: def cons_km(features, ml, k, ub = 6, MAX_ITERATIONS = 100, alpha = 0.5, c

        """Clustering with must-link constraints and upper bound for cluster

        Args:
            features: An array with shape (n_objects,n_features)
            mustlink: A list containing the pre-defined group, ex.[[a,b],[c,c
            k: Number of clusters
            ub: Upper bound for the cardinality of clusters.
            iterations: max number of iterations
            alpha

        Returns:
            k clusters.

        Raises:
            IOError: An error occurred when the given upper bound is not atta
        """

        ml.sort(key = len)
        ml = ml[::-1]
        lable = [None]*len(features)
        fix = []
        for group in ml:
            fix = fix + group
        free = [x for x in range(len(features)) if x not in fix]

        #initialize seeds
        if k > len(ml):
            for i in range(len(ml)):
                for member in ml[i]:
                    lable[member] = i
            centroids, lable = furthest_centroids(len(ml),k,lable,features)
        else:
```

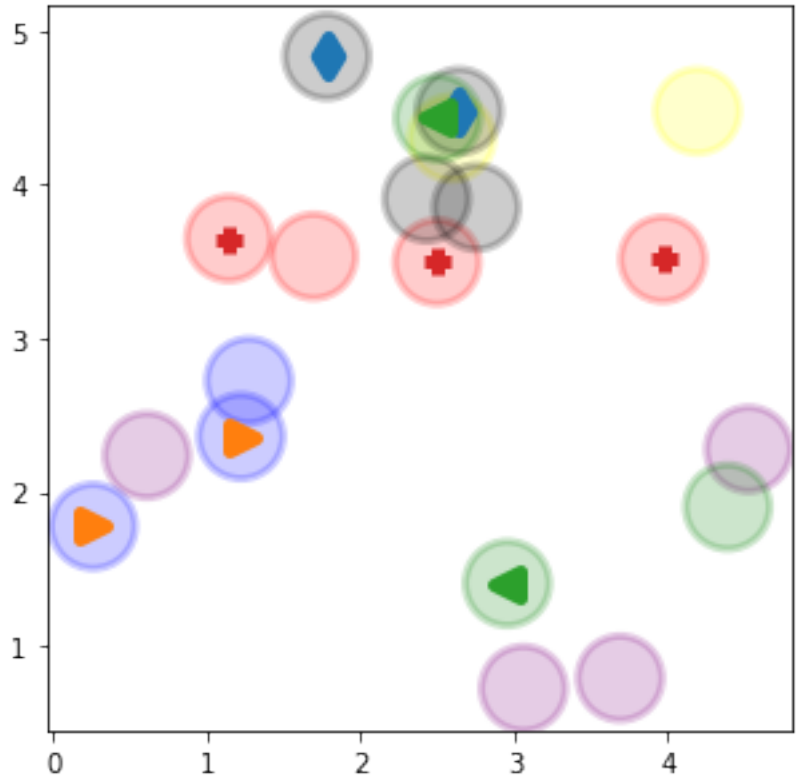
```
                for i in range(k):
                    for member in ml[i]:
                        lable[member] = i
                for i in range(k,len(ml)):
                    temp = fit_lable(ml[i],features,lable,ub,k)
                    for member in ml[i]:
                        lable[member] = temp
                centroids = get_centroids(features, lable, k)

            #k means:
            iterations = 0
            oldCentroids = None
            errors = []
            while not shouldStop(oldCentroids, centroids, iterations, alpha,MAX_I
                # Save old centroids for convergence test. Book keeping.
                oldCentroids = centroids
                iterations += 1
                #print(iterations)
                lable = get_lable(features, lable, centroids, free, ub, k)
                centroids = get_centroids(features, lable, k)
                if len(ground_truth)>0:
                    errors.append(clusters_error(lable,ground_truth))

            print('# of iterations:',iterations)
            return centroids,lable,errors
```

0.3 IV. Test on Randam data

In [7]:
```
# random generate 20 points
f = [[rd.uniform(0,5),rd.uniform(0,5)] for x in range(20)]
mlml = [[1,4,5],[6,7],[19,18],[12,13]]

#constraints-kmean
cen,lab = cons_km(features=f,ml=mlml,k=6,alpha=0.5,MAX_ITERATIONS=1000,ub=4

# visualize it
plt.figure(figsize=(5,5),)
colors = ['red', 'green','blue','black','yellow','purple']
plt.scatter([x[0] for x in f], [x[1] for x in f], s=1000, c=[colors[x] for

markers = ['x','+','<','>','d']
for group in mlml:
    temp = markers.pop()
    print(temp,group)
    plt.scatter([f[x][0] for x in group], [f[x][1] for x in group], s=100,l
plt.show()
```

```
3
```

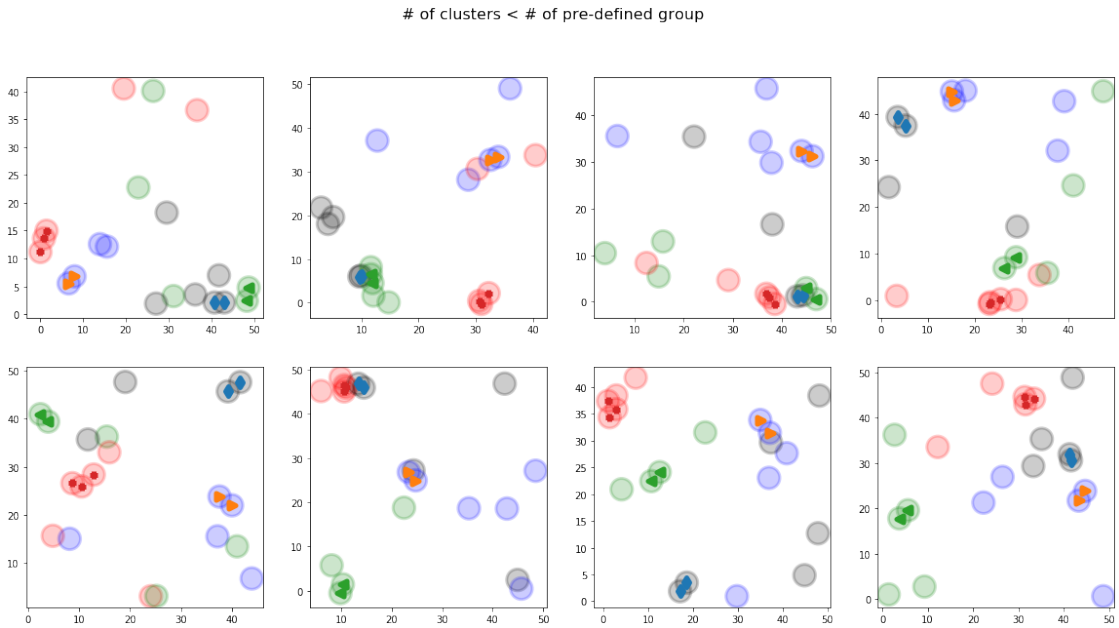
```
d [6, 7]
> [19, 18]
< [12, 13]
+ [1, 4, 5]
```



In [8]:
```
'''
Test on 20 data points
1.forced similarity within pre-fixed group
2.# of clusters < # of pre-defined group
'''

fig, ax = plt.subplots(nrows=2, ncols=4,figsize=(20,10))
fig.suptitle('# of clusters < # of pre-defined group', fontsize=16)

for row in ax:
    for col in row:
        #random generate 20 points
        f = [[rd.uniform(0,50),rd.uniform(0,50)] for x in range(20)]
        mlml = [[1,4,5],[6,7],[19,18],[12,13]]

        # make group similar:
```

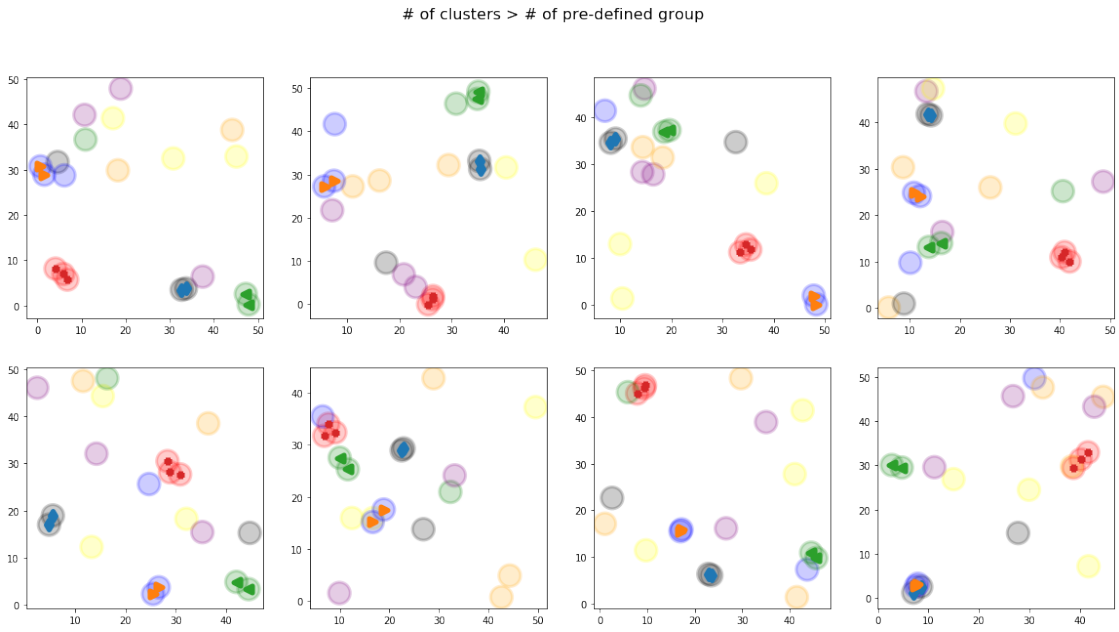
```
            for group in mlml:
                for i in range(1,len(group)):
                    f[group[i]][0] = f[group[0]][0] + rd.uniform(-2.5,2.5)
                    f[group[i]][1] = f[group[0]][1] + rd.uniform(-2.5,2.5)

            #constraints-kmean
            cen,lab = cons_km(features=f,ml=mlml,k=4,alpha=0.5,MAX_ITERATIONS=1

            # visualize it

            colors = ['red', 'green','blue','black']
            col.scatter([x[0] for x in f], [x[1] for x in f], s=500, c=[colors[

            markers = ['x','+','<','>','d']
            for group in mlml:
                temp = markers.pop()
                col.scatter([f[x][0] for x in group], [f[x][1] for x in group],

    plt.show()
```

```
1001
1001
1001
1001
1001
1001
1001
32
```



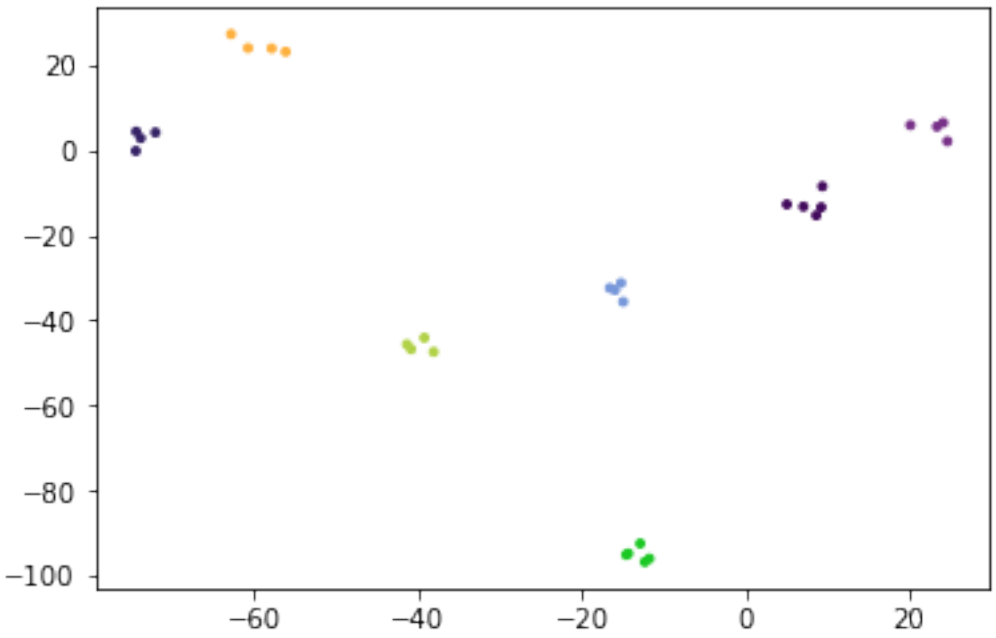
In [405]:
```
'''
Test on 20 data points with:
1.forced similarity within pre-fixed group
2.# of clusters > # of pre-defined group
'''

fig, ax = plt.subplots(nrows=2, ncols=4,figsize=(20,10))
fig.suptitle('# of clusters > # of pre-defined group', fontsize=16)

for row in ax:
    for col in row:
        #random generate 20 points
        f = [[rd.uniform(0,50),rd.uniform(0,50)] for x in range(20)]
        mlml = [[1,4,5],[6,7],[19,18],[12,13]]

        # make group similar:
        for group in mlml:
            for i in range(1,len(group)):
                f[group[i]][0] = f[group[0]][0] + rd.uniform(-2.5,2.5)
                f[group[i]][1] = f[group[0]][1] + rd.uniform(-2.5,2.5)

        #constraints-kmean
        cen,lab = cons_km(features=f,ml=mlml,k=7,alpha=0.5,MAX_ITERATIONS

        # visualize it

        colors = ['red', 'green','blue','black','purple','yellow','orange
        col.scatter([x[0] for x in f], [x[1] for x in f], s=500, c=[color

        markers = ['x','+','<','>','d']
        for group in mlml:
            temp = markers.pop()
            col.scatter([f[x][0] for x in group], [f[x][1] for x in group

plt.show()
```

```
1001
1001
1001
1001
1001
1001
1001
1001
```



0.4 V. Test on blob data

In [260]:
```
# generate data with ground true

import sklearn.datasets as sk_data

X, y = sk_data.make_blobs(n_samples=30, centers=7, n_features=2,
                          center_box=(-100.0, 100.0),random_state=2,clust
plt.scatter(X[:, 0], X[:, 1], s=8,c=[colors[x] for x in y])
plt.show()
```

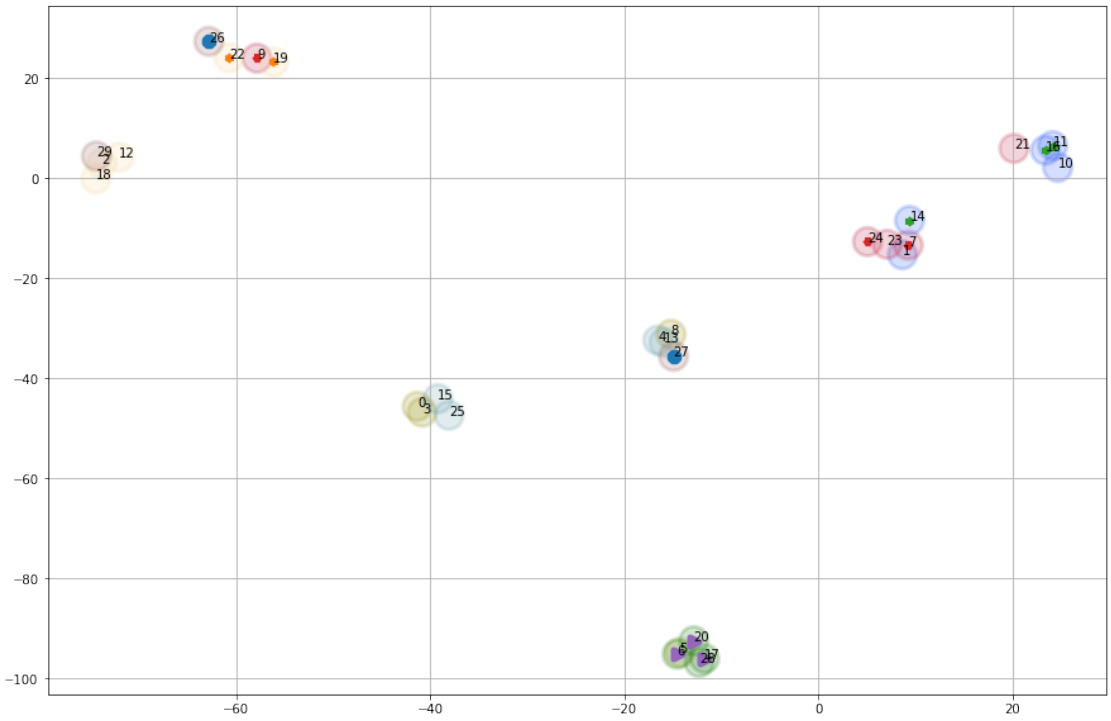


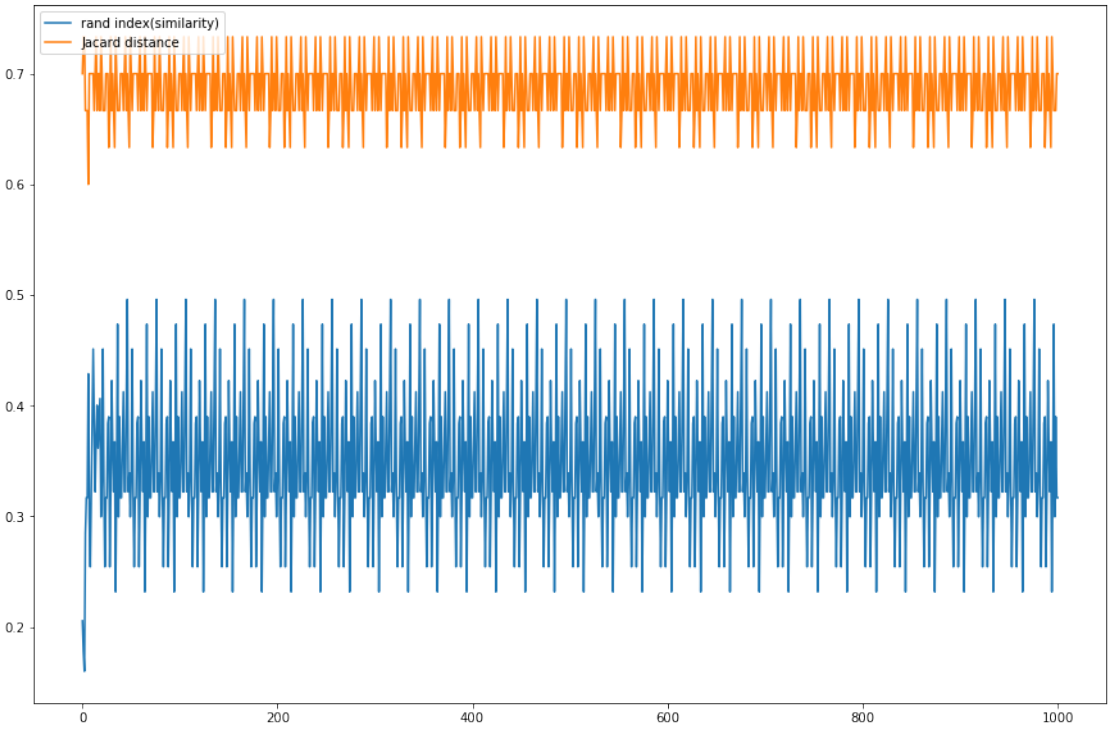

```
In [200]: # generate must-links
          def must_links_generators(X,k,lb,ub):
              """generates k pre-defined groups among the objects represented by X

              Args:
                  X: Objects matrix
                  k: Number of pre-defined groups
                  lb,ub: Size of group subjects to (lb,ub)
              Returns:
                  A 2d list that represents k pre-defined group.
              Raise:
                  IOError if cannot generate k satisfying groups
              """
              must_links = []
              pool = [x for x in range(len(X))]
              for i in range(k):
                  if len(pool) == 0: raise IOError("k or size too large")
                  rd.shuffle(pool)
                  size = rd.randint(2,4)
                  must_links.append(pool[-size:])
                  pool = pool[:-size]
              return must_links

          def clusters_error(lable,y):
              # rand index
              ri = metrics.adjusted_rand_score(lable,y)
```

```
        # jacard distance
        jd = sum([a!=b for (a,b) in zip(lable,y)])/len(y)
        return [ri,jd]
```

In [263]:
```
"""
Single test
"""
#constraints-kmean
mlml = must_links_generators(X,5,2,3)
f = X.tolist()
print('must_links:',mlml)
cen,lab,errors = cons_km(features=f,ml=mlml,k=7,alpha=0.01,MAX_ITERATIONS

# visualize plot
fig, ax = plt.subplots(figsize=(15,10))
r = lambda: rd.randint(0,255)
colors = ['#%02X%02X%02X' % (r(),r(),r()) for i in range(30)]

plt.scatter([x[0] for x in f], [x[1] for x in f], s=500, c=[colors[x] for

markers = ['x','+','<','1','d','>','2','3','4','8']
for group in mlml:
    temp = markers.pop()
    plt.scatter([f[x][0] for x in group], [f[x][1] for x in group], s=50,

for i, txt in enumerate(range(len(f))):
    ax.annotate(txt, (f[i][0],f[i][1]))

plt.grid()
plt.show()

# visualize error
plt.figure(figsize=(15,10))
l1, =plt.plot(range(len(errors)),[x[0] for x in errors],label ='rand inde
l2, = plt.plot(range(len(errors)),[x[1] for x in errors],label ='Jacard c
plt.legend(handles=[l1,l2], loc=2)
plt.show()
```

```
must_links: [[27, 26], [11, 14, 16], [9, 7, 24], [20, 6, 17], [19, 22]]
# of iterations: 1001
```

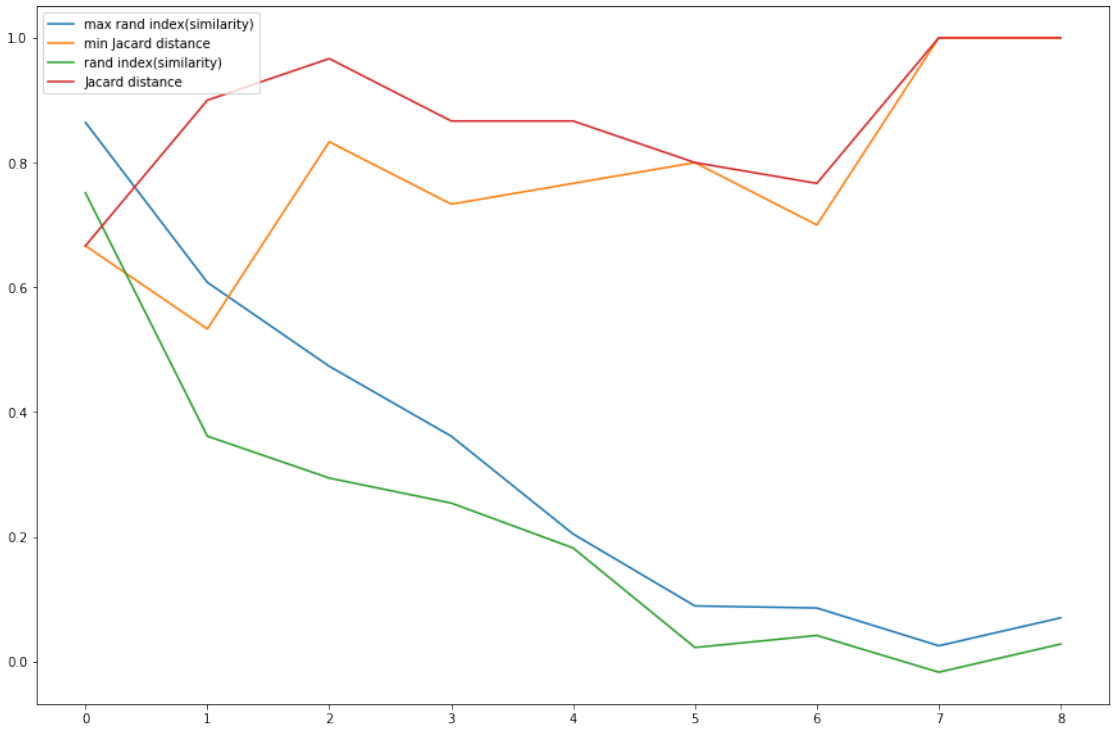

20
0
−20
−40
−60
−80
−100
−60
−40
−20
0
20


rand index(similarity)
Jacard distance
0.7
0.6
0.5
0.4
0.3
0.2
0
200
400
600
800
1000

In [268]:
```
"""
How error change as #constraints increases?
"""
for_plot  =[]
mlml = must_links_generators(X,9,2,3)
for i in range(9):
    f = X.tolist()
    print('must_links:',mlml[:i])
    cen,lab,errors = cons_km(features=f,ml=mlml[:i],k=7,alpha=0.01,MAX_IT
    max_sim = max([x[0] for x in errors])
    min_dis = min([x[1] for x in errors])
    for_plot.append((max_sim,min_dis,errors[-1][0],errors[-1][1]))
```

```
must_links: []
# of iterations: 1001
must_links: [[27, 12, 15]]
# of iterations: 1001
must_links: [[27, 12, 15], [0, 25, 11, 24]]
# of iterations: 1001
must_links: [[27, 12, 15], [0, 25, 11, 24], [26, 7, 2]]
# of iterations: 1001
must_links: [[27, 12, 15], [0, 25, 11, 24], [26, 7, 2], [5, 10, 17, 1]]
# of iterations: 1001
must_links: [[27, 12, 15], [0, 25, 11, 24], [26, 7, 2], [5, 10, 17, 1], [13, 20, 9,
# of iterations: 1001
must_links: [[27, 12, 15], [0, 25, 11, 24], [26, 7, 2], [5, 10, 17, 1], [13, 20, 9,
# of iterations: 1001
must_links: [[27, 12, 15], [0, 25, 11, 24], [26, 7, 2], [5, 10, 17, 1], [13, 20, 9,
# of iterations: 1001
must_links: [[27, 12, 15], [0, 25, 11, 24], [26, 7, 2], [5, 10, 17, 1], [13, 20, 9,
# of iterations: 1001
```

In [269]:
```
plt.figure(figsize=(15,10))
l1, =plt.plot(range(len(for_plot)),[x[0] for x in for_plot],label ='max r
l2, = plt.plot(range(len(for_plot)),[x[1] for x in for_plot],label ='min
l3, = plt.plot(range(len(for_plot)),[x[2] for x in for_plot],label ='rand
l4, = plt.plot(range(len(for_plot)),[x[3] for x in for_plot],label ='Jaca

plt.legend(handles=[l1,l2,l3,l4], loc=2)
plt.show()
```




```
In [210]: for i in range(12):
              print(sum(1 for x in lab if x == i))
```

```
4
5
4
5
5
5
4
4
2
3
4
5
```

```
In [ ]:
```