cluster_cdr_hamming

October 1, 2022

The routine, just copy-paste it

[122]:
```
import pandas as pd
import numpy as np
import igraph as ig
from scipy.spatial.distance import pdist, squareform
from plotnine import *

def seqs2hamming(seqs, threshold = 1):
    # pairwise hamming
    def hdist(s1, s2):
        if len(s1) != len(s2):
            return float('inf')
        else:
            return sum(c1 != c2 for c1, c2 in zip(s1, s2))

    seqs = np.array(seqs).astype("str")
    dm = squareform(pdist(seqs.reshape(-1, 1), metric = lambda x, y:␣
 ↪hdist(x[0], y[0])))
    dmf = pd.DataFrame(dm, index=seqs, columns=seqs).stack().reset_index()
    dmf.columns = ['id1','id2','distance']
    dmf = dmf[dmf['distance'] <= threshold]

    # graph
    graph = ig.Graph.TupleList(dmf[['id1', 'id2']].itertuples(index=False))

    # clusters
    clusters = graph.components()
    membership = clusters.membership

    # layout
    layout = graph.layout('graphopt')
    coords = np.array(layout.coords)

    df_graph = pd.DataFrame(
        {'cdr3': graph.vs()['name'],
         'cluster': membership,
         'x': coords[:,0],
```

```
        'y': coords[:,1]
    })

    # summary
    df_graph_summary = df_graph.groupby(['cluster']).agg(
        cluster_size = ('cluster', 'size'),
        x_mean = ('x', 'mean'),
        y_mean = ('y', 'mean')).reset_index()

    return pd.merge(df_graph, df_graph_summary)
```

Testing of A*02 GLC

[123]:
```
vdjdb = pd.read_csv('vdjdb.slim.txt', sep='\t')

def get_seqs(epi, gene = 'TRB'):
    return vdjdb[(vdjdb['antigen.epitope'] == epi) & (vdjdb['gene'] ==␣
 ↪gene)]['cdr3']

test_seqs = get_seqs('GLCTLVAML')

res = seqs2hamming(test_seqs)
res
```

[123]:

	cdr3	cluster	x	y	cluster_size	\
0	CASIPEGGRETQYF	0	-301.451313	-314.259030	1	
1	CASSEGRISPGELFF	1	135.129451	67.565574	12	
2	CASSEGRVSPGELFF	1	119.929664	88.846763	12	
3	CASSEGRVLSGELFF	1	103.324800	45.651130	12	
4	CASSEGRVLPGELFF	1	102.953739	69.861562	12	
..	…	…	…	…	…	
971	CAIEGGQSYEQYF	801	72.035140	531.144183	1	
972	CASSVGSNTGELFF	802	57.030601	-803.544736	1	
973	CASSFGATDTQYF	803	-322.101263	-70.680012	1	
974	CASSLSLHGNQPQHF	804	4.101026	372.554783	1	
975	CASSLEAADNYGYTF	805	-233.711827	174.656068	1	

	x_mean	y_mean
0	-301.451313	-314.259030
1	111.170383	90.515444
2	111.170383	90.515444
3	111.170383	90.515444
4	111.170383	90.515444
..	…	…
971	72.035140	531.144183
972	57.030601	-803.544736
973	-322.101263	-70.680012

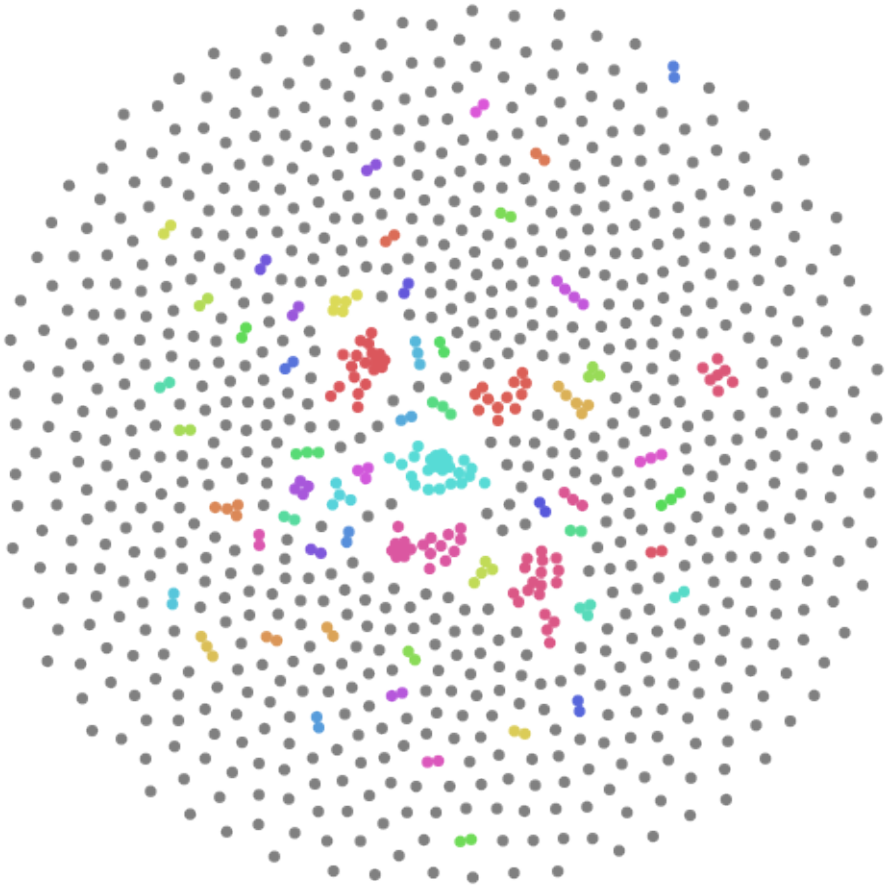
```
974    4.101026  372.554783
975 -233.711827  174.656068

[976 rows x 7 columns]
```

Write to file and plot

[124]:
```
res.to_csv("test_clusters.tsv", sep = "\t", index=False)

res['cc'] = res['cluster'].astype("str")
g = (ggplot(res[res['cluster_size'] > 1], aes(x='x', y='y', color='cc')) +
     geom_point(data = res[res['cluster_size'] == 1], color = 'grey') +
     geom_point() +
     scale_color_discrete(guide=False) +
     xlab('') +
     ylab('') +
     theme_void() +
     theme(aspect_ratio = 1))
print(g)
```



Now run it for groups - select epitopes with 500+ entries

[125]:
```
epitopes = test[(test['gene'] == 'TRB') & (test['antigen.epitope'] !=␣
↪'KLGGALQAK')]
epitopes = epitopes.groupby(['antigen.epitope']).agg(size = ('cdr3', 'size'))
epitopes = list(epitopes[epitopes['size'] >= 500].index)
len(epitopes)
```

[125]:
```
10
```

Build and concat matrices for all epitopes

[126]:
```
def fun2(epi):
    df = seqs2hamming(get_seqs(epi))
    df['group'] = epi
    return df

res2 = pd.concat([fun2(epi) for epi in epitopes])
res2
```

[126]:

	cdr3	cluster	x	y	cluster_size	\
0	CASSVTDRIRNTIYF	0	226.181376	535.269953	1	
1	CASSYLLAGLYNEQFF	1	-326.654995	22.099479	1	
2	CASRLSGSAYEQYF	2	-198.920217	912.073105	1	
3	CASSVTSSRGGTDTQYF	3	42.815817	757.878882	1	
4	CASSLSFRAHNEQFF	4	390.527926	341.570476	1	
..	…	…	…	…	…	
681	CSASDRRDEQFF	396	-527.146064	-290.316285	1	
682	CAIADANTGELFF	397	-410.043498	168.059475	1	
683	CAGLIMNTGELFF	398	-444.253797	204.848187	1	
684	CASSPEDTQYF	399	-336.954207	-529.799192	1	
685	CASSPRTATYEQYF	400	-217.920619	-266.739291	1	

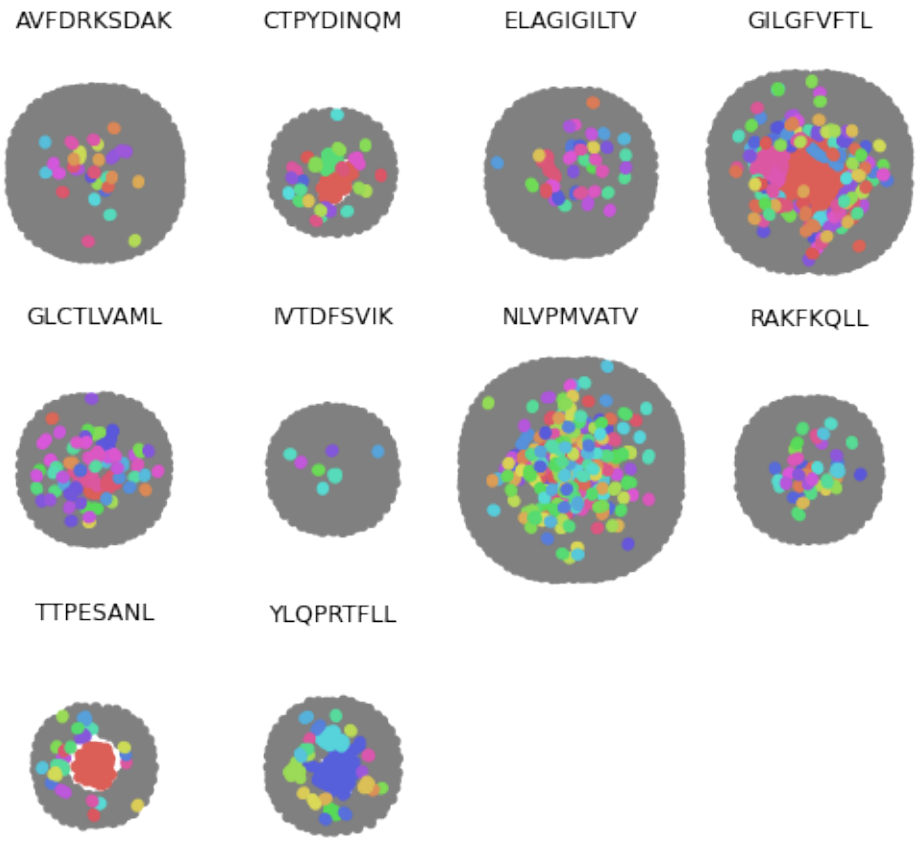
	x_mean	y_mean	group
0	226.181376	535.269953	AVFDRKSDAK
1	-326.654995	22.099479	AVFDRKSDAK
2	-198.920217	912.073105	AVFDRKSDAK
3	42.815817	757.878882	AVFDRKSDAK
4	390.527926	341.570476	AVFDRKSDAK
..	…	…	…
681	-527.146064	-290.316285	YLQPRTFLL
682	-410.043498	168.059475	YLQPRTFLL
683	-444.253797	204.848187	YLQPRTFLL
684	-336.954207	-529.799192	YLQPRTFLL

```
685 -217.920619 -266.739291   YLQPRTFLL

[15284 rows x 8 columns]
```

Plot

[127]:
```
res2['cc'] = res2['cluster'].astype("str")
g2 = (ggplot(res2[res2['cluster_size'] > 1], aes(x='x', y='y', color='cc')) +
     geom_point(data = res2[res2['cluster_size'] == 1], color = 'grey') +
     geom_point() +
     scale_color_discrete(guide=False) +
     xlab('') +
     ylab('') +
     facet_wrap('group') +
     theme_void() +
     theme(aspect_ratio = 1))
print(g2)
```



[ ]: