In [1]:

```
import os
import numpy as np
import networkx as nx
from networkx.algorithms.components import connected_components as connected_components
import pickle
import matplotlib.pyplot as plt
from scipy.stats import ks_2samp
#
DATA_FOLDER = 'data/'
```

In [2]:

```
def get_random_connected_motif(nodes_per_graph,num_edges,random_motif_size):
    if random_motif_size:
        num_edges = np.random.randint(2,num_edges+1)
    min_nodes = int(np.ceil((1+np.sqrt(1+8*num_edges))/2))
    num_nodes = np.random.randint(min_nodes,num_edges+2)
    while True:
        tmp = nx.empty_graph()
        edges = [(a,b) for a in range(num_nodes) for b in range(a+1,num_nodes)]
        assert len(edges) >= num_edges
        while True:
            n1,n2 = edges[np.random.randint(len(edges))]
            tmp.add_edge(n1,n2)
            edges.remove((n1,n2))
            if len(tmp.edges)==num_edges:
                break
        if nx.is_connected(tmp):
            node_ids = np.random.choice(range(nodes_per_graph),len(tmp),replace=False)
            tmp = nx.relabel.relabel_nodes(tmp,dict(zip(range(nodes_per_graph),node_ids)))
            return tmp
```

In [3]:

```
def add_pattern_inplace(graph,motif):
    for edge in motif.edges:
        graph.add_edge(*edge)

def remove_pattern_inplace(graph,motif):
    for edge in motif.edges:
        if edge in graph.edges:
            graph.remove_edge(*edge)
```

In [4]:

```
def mutate(base_graph,perturbation_prob,motifs_to_add,motifs_to_remove):
    new_graph = base_graph.copy()
    for motif in motifs_to_add:
        if np.random.rand()<perturbation_prob:
            add_pattern_inplace(new_graph,motif)
    for motif in motifs_to_remove:
        if np.random.rand()<perturbation_prob:
            remove_pattern_inplace(new_graph,motif)
    return new_graph
```

In [5]:

```
def plot_motifs(motifs,num_cols=5):
    num_rows = len(motifs)//num_cols
    plt.figure(figsize=(16,3*num_rows))
    for indx,g in enumerate(motifs):
        plt.subplot(num_rows,num_cols,indx+1)
        nx.draw_networkx(g,node_color='orangered' if indx%2==0 else 'dod
gerblue')
        plt.title(str(len(list(g.edges)))+' edges, class '+str(indx%2))
```

In [6]:

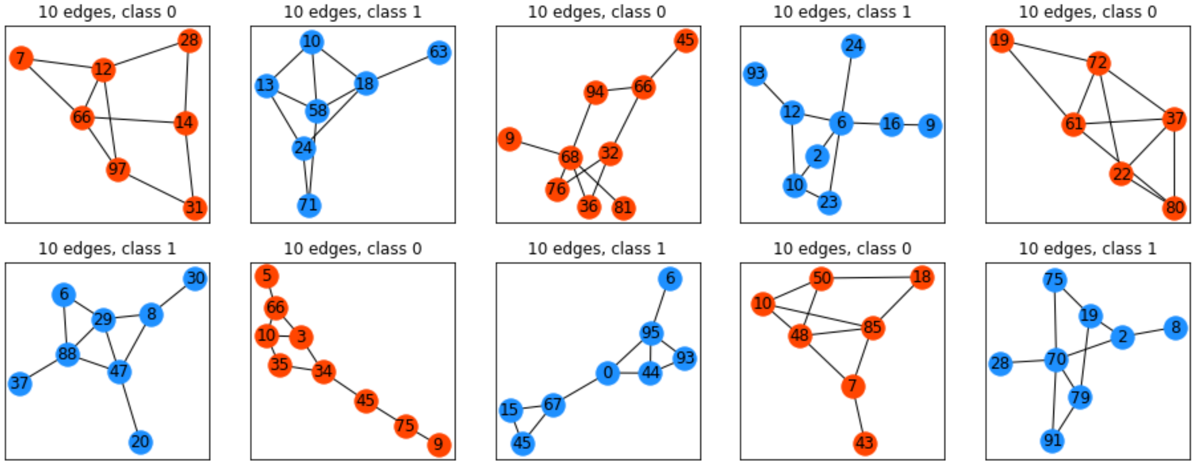
```
def make_base_graph(nodes_per_graph,graph_density):
    base_graph = nx.empty_graph()
    for node in range(nodes_per_graph):
        base_graph.add_node(node)
    for edge in nx.erdos_renyi_graph(nodes_per_graph,graph_density).edge
s:
        base_graph.add_edge(*edge)
    return base_graph
```

In [7]:

```
def make_dataset(graphs_per_class,nodes_per_graph,graph_density,
                        motif_num,motif_size,random_motif_size,perturbat
ion_prob):
    motifs = [get_random_connected_motif(nodes_per_graph,motif_size,rand
om_motif_size) for _ in range(motif_num)]
    motifs = sorted(motifs, key=lambda m: len(m.edges))
    motifs_0 = motifs[0::2]
    motifs_1 = motifs[1::2]
    #
    graphs_0 = [mutate(make_base_graph(nodes_per_graph,graph_density),pe
rturbation_prob,\
                          motifs_0,motifs_1) for _ in range(graphs_per_c
lass)]
    graphs_1 = [mutate(make_base_graph(nodes_per_graph,graph_density),pe
rturbation_prob,\
                          motifs_1,motifs_0) for _ in range(graphs_per_c
lass)]
    return graphs_0,graphs_1,motifs
```

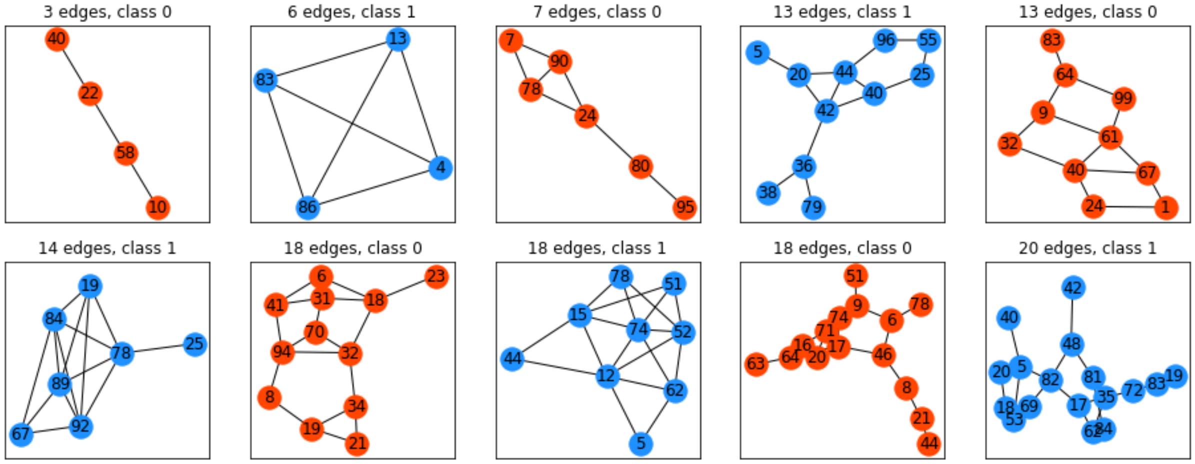
In [8]:

```
#Generate small dataset with fixed motif size
graphs_0,graphs_1,motifs = make_dataset(graphs_per_class=100,nodes_per_graph=100,graph_density=.2,\
                    motif_num=10,motif_size=10,random_motif_size=False,perturbation_prob=.5)
plot_motifs(motifs)
```



In [9]:

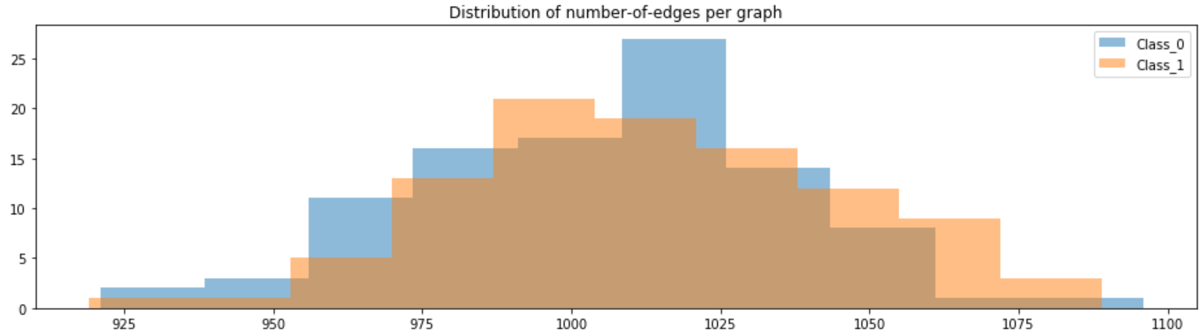
```
#Generate small dataset with variable motif size
graphs_0,graphs_1,motifs = make_dataset(graphs_per_class=100,nodes_per_graph=100,graph_density=.2,\
                    motif_num=10,motif_size=20,random_motif_size=True,perturbation_prob=.5)
plot_motifs(motifs)
```



```
In [10]: def check_classes(graphs_0,graphs_1):
             num_nodes = len(graphs_0[0])
             for graphs_class,class_label in zip([graphs_0,graphs_1],['class_0',
         'class_1']):
                 class_density = np.mean([len(g.edges)/(num_nodes*num_nodes/2) fo
         r g in graphs_class])
                 class_unique = len(set([a for b in [g.edges for g in graphs_clas
         s] for a in b]))
                 print(class_label,len(graphs_class),'elems,',class_unique,'uniqu
         e edges - density',class_density)
             plt.figure(figsize=(16,4))
             plt.hist([len(g.edges) for g in graphs_0],alpha=.5,label='Class_0')
             plt.hist([len(g.edges) for g in graphs_1],alpha=.5,label='Class_1')
             plt.legend()
             plt.title('Distribution of number-of-edges per graph')
```

```
In [11]: check_classes(graphs_0,graphs_1)
```

```
class_0 100 elems, 4950 unique edges - density 0.20105599999999998
class_1 100 elems, 4950 unique edges - density 0.202722
```



```
In [12]: #generate and save a dataset
         graphs_0,graphs_1,motifs = make_dataset(graphs_per_class=100,nodes_per_g
         raph=100,graph_density=.2,\
                             motif_num=5,motif_size=10,random_motif_size=False,pe
         rturbation_prob=.2)
         #
         dump_name = 'p20s10n05'
         pickle.dump(graphs_0, open(DATA_FOLDER+'synth_'+dump_name+'_0','wb'))
         pickle.dump(graphs_1, open(DATA_FOLDER+'synth_'+dump_name+'_1','wb'))
         pickle.dump(motifs,open(DATA_FOLDER+'injected_'+dump_name,'wb'))
```

Experiment 5.1

In [13]:

```
def jaccard_distance_function(graphA,graphB):
    edgesA,edgesB = graphA.edges,graphB.edges
    intersection = len(set(edgesA).intersection(set(edgesB)))
    union = len(set(edgesA).union(set(edgesB)))
    return 1-intersection/union

def jaccard_matrix(graphs_0,graphs_1):
    dataset = graphs_0+graphs_1
    total_size = len(dataset)
    jaccard_distance_matrix = np.full((total_size,total_size),-1,dtype=f
loat)
    for i in range(total_size):
        for j in range(total_size):
            if j>i:
                jaccard_distance_matrix[i][j] = jaccard_distance_functio
n(dataset[i],dataset[j])
    return jaccard_distance_matrix

def get_ks(graphs_0,graphs_1):
    jaccard_distance_matrix = jaccard_matrix(graphs_0,graphs_1)
    total_size = len(graphs_0+graphs_1)
    mid_point = len(graphs_0)
    same_distr = [jaccard_distance_matrix[i][j] for i in range(total_siz
e) for j in range(total_size) \
                                               if j>i and not (i<mid_poin
t and j>=mid_point)]
    diff_distr = [jaccard_distance_matrix[i][j] for i in range(mid_point
) for j in range(mid_point,total_size)]
    return ks_2samp(same_distr,diff_distr)[0]
```

In [14]:

```
def batch_measure_separability(graphs_per_class,nodes_per_graph,graph_de
nsity,\
                              motif_num_values,motif_size_values,perturb
ation_prob_values):
    logger = {}
    print('TOTAL',len(motif_num_values)*len(motif_size_values)*len(pertu
rbation_prob_values),'experiments')
    indx = 0
    for motif_num in motif_num_values:
        for motif_size in motif_size_values:
            for perturbation_prob in perturbation_prob_values:
                print(indx,end=' ')
                ks_scores = []
                for _ in range(30):
                    graphs_0,graphs_1,motifs = make_dataset(graphs_per_c
lass,nodes_per_graph,\
                                graph_density,motif_num,motif_size,False
,perturbation_prob)
                    ks_scores.append(get_ks(graphs_0,graphs_1))
                logger[(motif_num,motif_size,perturbation_prob)] = ks_sc
ores
                indx+=1
    return logger
```

In [15]:

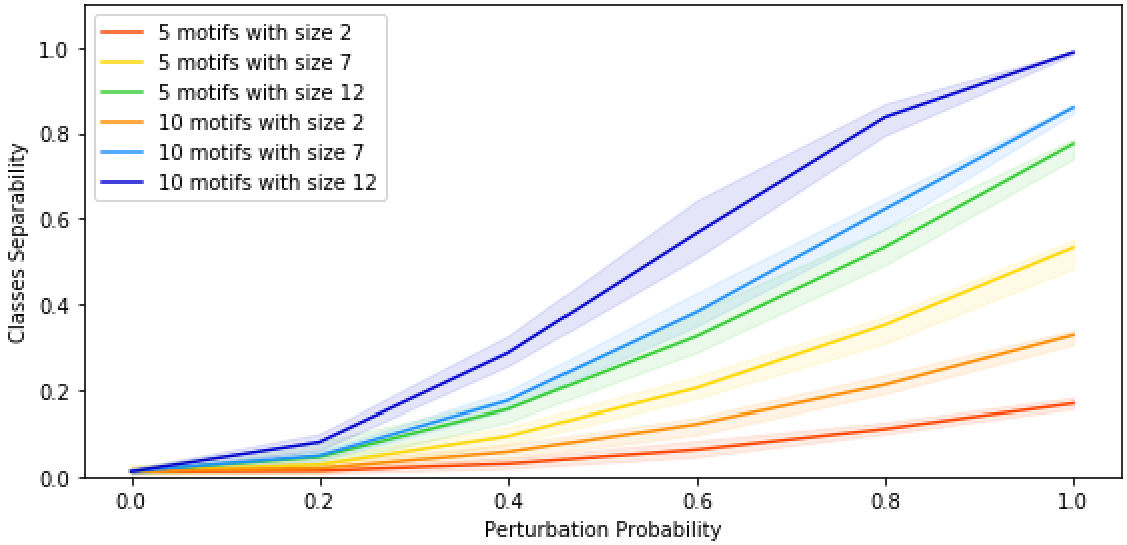
```
rerun_experiment = False
if rerun_experiment:
    logger = batch_measure_separability(graphs_per_class=100,nodes_per_graph=100,graph_density=.2,\
            motif_num_values=[5,10],motif_size_values=[2,7,12],perturbation_prob_values=[0,.2,.4,.6,.8,1])
    pickle.dump(logger,open(DATA_FOLDER+'logger','wb'))
else:
    logger = pickle.load(open(DATA_FOLDER+'logger','rb'))
```

In [16]:

```
def plot_separability(logger):
    plt.figure(figsize=(8,4))
    ycolors = ['orangered','gold','limegreen','darkorange','dodgerblue','mediumblue']
    motif_num_values = sorted(list(set([k[0] for k in logger.keys()])))
    motif_size_values = sorted(list(set([k[1] for k in logger.keys()])))
    perturbation_prob_values = sorted(list(set([k[2] for k in logger.keys()])))
    for indx,(mn,ms) in enumerate([(mn,ms) for mn in motif_num_values for ms in motif_size_values]):
        yavg = [np.mean(logger[(mn,ms,itrx)]) for itrx in perturbation_prob_values]
        ymax = [np.max(logger[(mn,ms,itrx)]) for itrx in perturbation_prob_values]
        ymin = [np.min(logger[(mn,ms,itrx)]) for itrx in perturbation_prob_values]
        ycolor = ycolors[indx%(len(ycolors))]
        plt.plot(perturbation_prob_values, yavg, label=str(mn)+' motifs with size '+str(ms), color=ycolor)
        plt.fill_between(perturbation_prob_values, ymin, ymax, alpha=0.1, edgecolor=ycolor, facecolor=ycolor)
    plt.xlabel('Perturbation Probability')
    plt.ylabel('Classes Separability')
    plt.ylim(top=1.1,bottom=0)
    plt.legend()
    plt.tight_layout()
```

In [17]:

```
plot_separability(logger)
```



In [ ]:

```
```