import

```
In [2]: import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns
import os
import time
import pickle
from sklearn.preprocessing import MinMaxScaler
In [7]: current_dir = os.getcwd()
file_dir=os.path.join(current_dir, "import_data\EV_data.xlsx") # file dir
df_import = pd.read_excel(file_dir, index_col=0, sheet_name=None)
df_import
```

global function

```
In [ ]: def moving_avg(dataframe, n=10, skip='PS', random_state=42):
            df = dataframe.copy(deep=True)
            df['type'] = [i.split('_')[0] for i in df.index]
            temp=pd.DataFrame()
            if skip != None:
                temp = df.query('type == @skip').copy(deep=True)
            df drop = df.drop(index=df[df['type']=='PS'].index)
            df_moving_avg = pd.DataFrame()
            for i in df_drop['type'].unique():
                df_i = df_drop.query('type == @i').drop(columns=['type'])
                df_i_shuffle = df_i.sample(frac=1, random_state=random_state,
                                            axis=0) #randomly take frac% from all; axis=0, row;
                j=0
                while j+n <= len(df_i_shuffle):</pre>
                    df mean = pd.DataFrame(df i shuffle.iloc[j:j+n,:].mean()).T
                    df mean['type'] = i
```

```
df moving avg = pd.concat([df moving avg, df mean])
                    j += 1
            df moving avg = pd.concat([df_moving_avg, temp])
            return of moving avg
In [2]: from sklearn.ensemble import RandomForestClassifier
        from sklearn.model selection import StratifiedShuffleSplit
        def split train test(dataframe, y col='type num', split y=False, cut=['type num','type'], test size=0.25, random state=42):
            'split trainset & test set'
            split = StratifiedShuffleSplit(test size=test size, random state=random state)
            for train index, test index in split.split(dataframe, dataframe[y col]):
                train set = dataframe.iloc[train index]
                test set = dataframe.iloc[test index]
            if split y == True:
                df_train_x, df_train_y = num_cut(train_set, cut)
                df test x, df test y = num cut(test set, cut)
                return df train x, df train y[y col], df test x, df test y[y col]
            elif split y == False:
                return train_set, test_set
        def num cut(dataframe, columns):
            'split number & str type'
            data cat = dataframe.loc[:, columns]
            data_num = dataframe.drop(columns=columns)
            return data_num, data_cat
In [ ]: def conf_mat_heatmap(conf_mat, rect_set, title, ticklabel=['A549','MCF10A','MCF7','PS'], cmap=None, mask=None):
            fig = plt.figure(dpi=130, figsize=(2.5,2.5))
            ax1 = fig.add subplot(111)
            density_mat = conf_mat/np.sum(conf_mat, axis=1).reshape(conf_mat.shape[0], -1)
            if cmap == None:
                cmap = sns.cubehelix palette(rot=0.2, gamma=0.5, dark=0.3, light=1, as cmap=True)#return matplotlib colormap
            elif cmap == '5imp':
                cmap = LinearSegmentedColormap.from list(name='cmap', colors=['w','orange'])
            if mask == True:
                mask=np.array(density mat==0)
            h = sns.heatmap(data=density_mat, xticklabels=ticklabel, yticklabels=ticklabel, annot = True,
                            fmt=".1%", linewidths=1, linecolor="0.7", cbar=False, #turn off color bar
                            annot kws={'size':10,'weight':600,'family':"Arial",'color':"k"},
                            square=True, vmin=0, vmax=1, cmap=cmap, ax=ax1, mask=mask)
```

```
ax1.tick params(width=2, length=4, colors="k")
    rect = plt.Rectangle(xy=rect set["xy1"], width=rect set["width1"], height=rect set["height1"],
                         fill=False, edgecolor="k", linewidth=rect set["linewidth1"])
    ax1.add patch(rect)
   # color bar
    rect cb = [1, 0.13, 0.11, 0.74]
   cbar ax = fig.add axes(rect cb)
    cb = h.figure.colorbar(h.collections[0], cax=cbar ax) #show colorbar
   cb.ax.tick_params(direction='in', labelsize=10, length=4, width=1, colors="k",
                      left=True, right=True)
    rect2 = plt.Rectangle(xy=rect set["xy2"], width=rect set["width2"], height=rect set["height2"],
                        fill=False, edgecolor="k", linewidth=rect set["linewidth2"] )
    cbar ax.add patch( rect2 )
   # title
   font1 = {'family':'Arial', 'color':'k', 'weight':'bold', 'size': 12}
    accu = conf mat.trace()/conf mat.sum()
   ax1.set xlabel('Accuracy Score:{:.1%}'.format(accu), font1);
   ax1.set ylabel("Actual", font1);
    ax1.set title(str(title)+'\n Predicted', font1);
rect_set2={"xy1":(0.023,0.017), "width1":2.94, "height1":2.96,"linewidth1":2.2,
                    "xy2":(0.03,0.004), "width2":0.97, "height2":0.99, "linewidth2":1.1}
rect set3={"xy1":(0.03,0.017), "width1":3.94, "height1":3.96, "linewidth1":1.5,
                    "xy2":(0.03,0.002), "width2":0.97, "height2":1,"linewidth2":1.1}
```

moving_average with RF

```
In [3]: from sklearn.metrics import confusion_matrix
from sklearn.metrics import accuracy_score
from sklearn.model_selection import cross_val_predict

def ML_result(ML, X, y, X_test, y_test):
    "input: ML algorithm. autofit, then output confusion_matrix & accuracy."
    ML.fit(X, y) #fit
    #train
    y_pred = cross_val_predict(ML, X, y, cv=3)
    confmat_train = confusion_matrix(y, y_pred)
    accu_train = accuracy_score(y, y_pred)
    impo = ML.feature_importances_
```

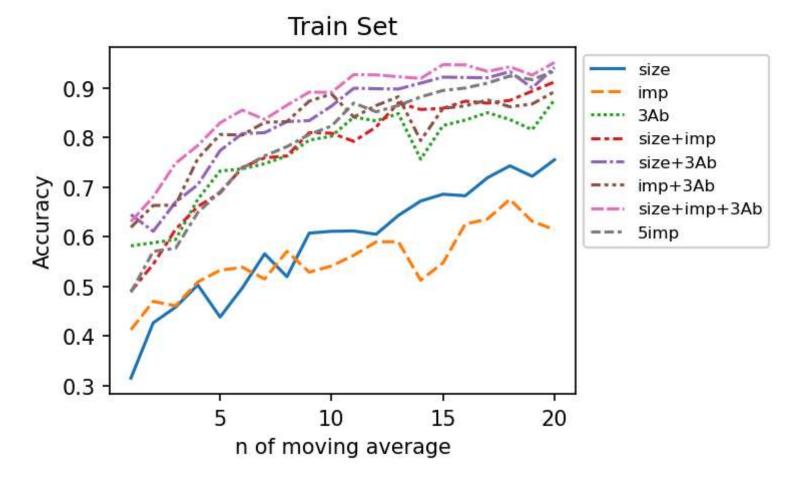
```
impo df = pd.DataFrame(sorted(zip(impo, X.columns), reverse=True))
            #test
            final pred = ML.predict(X test)
            confmat test = confusion matrix(y test, final pred)
            accu test = accuracy score(y test, final pred)
            return {"confmat train":confmat train, "accu train":accu train,
                    'confmat test':confmat test, "accu test":accu test, 'feature importance':impo df}
In [ ]: from sklearn.preprocessing import MinMaxScaler
        type 2 num={'A549':0, 'MCF10A':1, 'MCF7':2, 'PS':3}
        def find best n(data dict, n range, skip mov='PS', skip norm='5imp', random state=42):
            'moving average, then normalize'
            accu train = pd.DataFrame(np.zeros([len(n_range),len(data_dict)]), index = n_range,
                                      columns = data dict.keys()) #empty, accuracy of train set
            accu test = pd.DataFrame(np.zeros([len(n range),len(data dict)]), index = n range,
                                      columns = data dict.keys()) #accuracy of test set
            result = {}
            for key in data dict:
                result n = []
                for n in n range:
                    data_mov = moving_avg(data_dict[key], n=n, skip=skip_mov, random state=random state)
                    data mov['type num'] = [type 2 num[i] for i in data mov['type']]
                    if key != skip norm:
                        temp = data mov.loc[:,['type num','type']].copy(deep=True)
                        df drop = data mov.drop(columns=['type num', 'type'])
                        df normalized = MinMaxScaler((0,1)).fit transform(df drop)
                        df processed = pd.DataFrame(df normalized, columns=df drop.columns, index=df drop.index)
                        df avg norm = pd.concat([df processed, temp], axis=1)
                    else:
                        df avg norm = data mov.copy(deep=True)
                    df train x, df train y, df test x, df test y = split train test(df avg norm, y col='type num', split y=True)
                    forest clf = RandomForestClassifier(n jobs=-1, random state=random state, n estimators=100)
                    clf result = ML result(forest clf, df train x, df train y, df test x, df test y)
                    result n += [clf result]
                    accu_train.loc[n, key] = clf_result["accu_train"]
                    accu_test.loc[n, key] = clf_result["accu_test"]
```

result[key] = result n

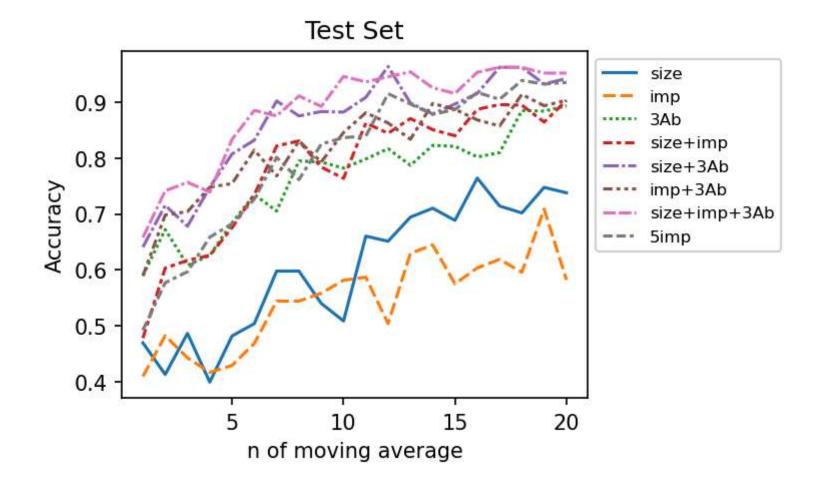
return result, accu train, accu test

```
In [767...
          result rf, accu train rf, accu test rf = find best n(df import, n range=range(1,21))
          current dir = os.getcwd()
          root_dir=os.path.join(current_dir, "export_data\moving_avg_RF")
          run id = time.strftime("%Y %m %d %H %M %S ")
          accu_train_rf.to_excel(os.path.join(root_dir, run_id+'accu_train.xlsx'))
          accu_test_rf.to_excel(os.path.join(root_dir, run_id+'accu_test.xlsx'))
          with open(os.path.join(root dir, run id+'result.pickle'), 'wb') as f:
              pickle.dump(result_rf, f)
In [769... fig, ax1 = plt.subplots(figsize=(4,3), dpi=150)
          sns.lineplot(accu_train_rf)
          ax1.set_ylabel('Accuracy',)
          ax1.set_xlabel('n of moving average',)
          #plt.ylim([0.3,1.05])
          plt.title('Train Set');
          plt.legend(bbox_to_anchor=(1,1), loc='upper left', fontsize=8, frameon=True, ncol=1)
```

Out[769... <matplotlib.legend.Legend at 0x1f407282040>



Out[770... <matplotlib.legend.Legend at 0x1f3cc266490>



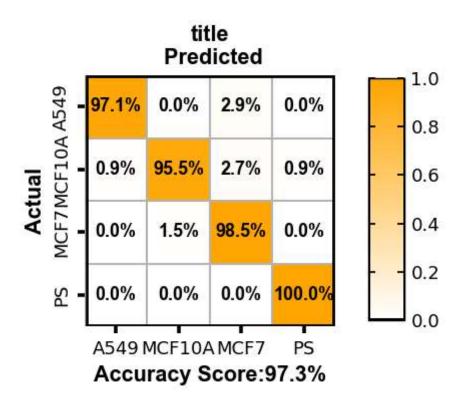
export_data

```
with pd.ExcelWriter(test file path, mode='w', engine='openpyxl') as writer:
                  empty.to excel(writer, sheet name='sheet1')
              for key in result:
                  with pd.ExcelWriter(train file path, mode='a', engine='openpyxl') as writer:
                      confmat train = pd.DataFrame(result[key][n-1]['confmat train'], columns=tick label, index=tick label)
                      confmat train.to excel(writer, sheet name=key)
                  with pd.ExcelWriter(test file path, mode='a', engine='openpyxl') as writer:
                      confmat test = pd.DataFrame(result[key][n-1]['confmat test'], columns=tick label, index=tick label)
                      confmat test.to excel(writer, sheet name=key)
              if impo ==True:
                  with pd.ExcelWriter(impo file path, mode='w', engine='openpyxl') as writer:
                      result['size+imp+3Ab'][n-1]['feature importance'].to excel(writer, sheet name='size+imp+3Ab')
                      result['5imp'][n-1]['feature importance'].to excel(writer, sheet name='5imp')
         #export confmat
In [772...
          root dir=os.path.join(current dir, "export data\moving avg RF")
          run id = time.strftime("%Y %m %d %H %M %S")
          export data(result rf, root dir=root dir, n=10, impo=True, file name='confmat '+run id+'.xlsx')
In [853...
         #export moving ava
          name=['size+imp+3Ab', 'size+imp', 'size+3Ab', 'imp+3Ab', 'size', 'imp', '3Ab', '5imp']
          ex dir=os.path.join(current dir, "export data\moving avg export data")
          for item in name:
              data_mov = moving_avg(df_import[item], n=10, skip='PS', random_state=42)
              data mov['type num'] = [type 2 num[i] for i in data mov['type']]
              temp = data_mov.loc[:,['type_num','type']].copy(deep=True)
              df drop = data mov.drop(columns=['type num', 'type'])
              df normalized = MinMaxScaler((0,1)).fit transform(df drop)
              df_processed = pd.DataFrame(df_normalized, columns=df_drop.columns, index=df_drop.index)
              df avg norm = pd.concat([df processed, temp], axis=1)
              df avg norm.to excel(os.path.join(ex dir,item+' n=10.xlsx'))
```

plot

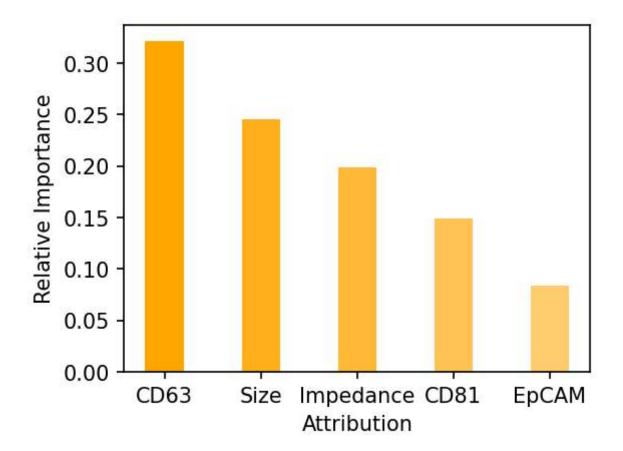
```
for key in result:
                  for item in name:
                      conf mat heatmap(result[key][n-1][item list[item]], rect set=rect set, cmap=cmap,
                                       title=item, ticklabel=tick label)
                  if impo==True:
                      draw impo(result[key][n-1]['feature importance'], cmap=cmap)
In [775...
         from matplotlib.colors import LinearSegmentedColormap
          impo label={'CD63 contrast change':'CD63','Size/nm':'Size', 'Imp contrast change':'Impedance',
                      'CD81 contrast change':'CD81', 'EpCAM contrast change':'EpCAM'}
          def draw impo(impo df, cmap=None):
              fig, ax1 = plt.subplots(figsize=(4,3), dpi=150)
              if cmap == None:
                  cmap = sns.cubehelix palette(rot=0.2, gamma=0.5, dark=0.3, light=1, n colors=10, reverse=True)
              elif cmap == '5imp':
                  cmap = LinearSegmentedColormap.from list(name='cmap',colors=['orange','w'], N=10)(range(10))
              ax1.bar(x=impo df[1], height=impo df[0], width=0.4, color=cmap,)#edgecolor='coral'
              ax1.set ylabel('Relative Importance')
              ax1.set xlabel('Attribution')
              if ax1.get xticklabels()[0].get text() != '45Hz':
                  curr label = [impo label[item.get text()] for item in ax1.get xticklabels()]
                  ax1.set xticklabels(curr label, rotation=0, fontsize=10)
 In [ ]: data mov = moving_avg(df_import['size+imp+3Ab'], n=10, skip='PS', random_state=42)
          data mov['type num'] = [type 2 num[i] for i in data mov['type']]
          temp = data mov.loc[:,['type num','type']].copy(deep=True)
          df drop = data mov.drop(columns=['type num', 'type'])
          df_normalized = MinMaxScaler((0,1)).fit_transform(df_drop)
          df_processed = pd.DataFrame(df_normalized, columns=df_drop.columns, index=df drop.index)
          df_avg_norm = pd.concat([df_processed, temp], axis=1)
          df train x, df train y, df test x, df test y = split train test(df avg norm, y col='type num', split y=True)
          forest clf = RandomForestClassifier(n jobs=-1, random state=42, n estimators=100)
          #clf result = ML result(forest clf, df train x, df train y, df test x, df test y)
          forest clf.fit(df train x, df train y) #fit
          #train
          y pred = cross val predict(forest clf, df train x, df train y, cv=3)
          confmat train = confusion matrix(df train y, y pred)
          accu train = accuracy score(df train y, y pred)
```

```
impo = forest clf.feature importances
         impo df = pd.DataFrame(sorted(zip(impo, df train x.columns), reverse=True))
          #test
         final pred = forest clf.predict(df test x)
         confmat test = confusion matrix(df test y, final pred)
         accu test = accuracy score(df test y, final pred)
         clf result = {"confmat train":confmat train, "accu train":accu train,
                         'confmat test':confmat test, "accu test":accu test, 'feature importance':impo df}
 In [ ]: clf result
 Out[]: {'confmat_train': array([[ 66, 0, 2, 0],
                 [ 1, 107, 3, 1],
                 [ 0, 2, 132, 0],
                 [ 0, 0, 0, 15]], dtype=int64),
           'accu train': 0.9726443768996961,
           'confmat test': array([[22, 0, 1, 0],
                 [ 0, 34, 3, 0],
                 [ 0, 0, 45, 0],
                 [ 0, 0, 0, 5]], dtype=int64),
           'accu test': 0.9636363636363636,
           'feature importance':
                                                               1
           0 0.321476 CD63_contrast_change
           1 0.246028
                                     Size/nm
           2 0.199100 Imp contrast change
           3 0.149314 CD81 contrast change
           4 0.084082 EpCAM_contrast_change}
In [586... conf_mat_heatmap(clf_result['confmat_train'], rect_set3, 'title', cmap='5imp')
```



In [684... draw_impo(clf_result['feature_importance'], cmap='5imp')

C:\Users\DELL\AppData\Local\Temp\ipykernel_5676\2762760416.py:15: UserWarning: FixedFormatter should only be used together with FixedLocator ax1.set xticklabels(curr label, rotation=0, fontsize=10)



```
In [12]: draw_selected_confmat(result_rf, 10, name=['Training Set','Test Set'], impo=True, cmap=None)
```

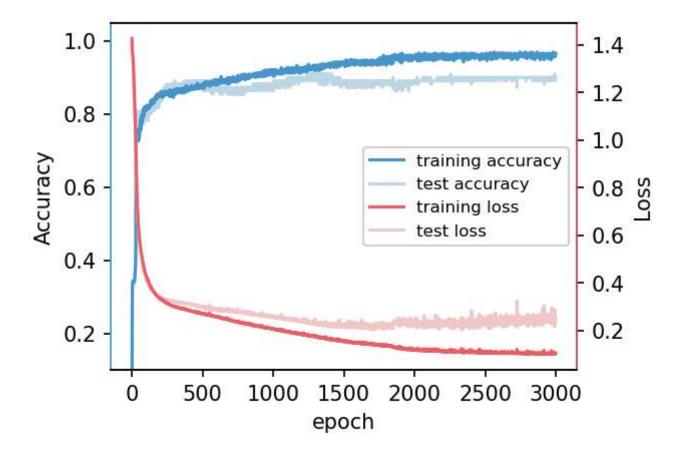
moving_average with DNN

func

```
model = tf.keras.models.Sequential()
              model.add(tf.keras.layers.InputLayer(input shape=input shape)) #InputLayer, shape(None, 5)
              for neurons in Dense config['Dense']:
                  model.add(tf.keras.layers.Dense(neurons, activation='relu'))
              model.add(tf.keras.layers.Dense(output, activation='softmax'))
              return model
          #model.get config()
          #modeL.summary()
          #model.save("my model.h5") #save as HDF5
          #model = tf.keras.models.load model("my model.h5")
 In [11]: def run model(model, data mov, lr 0=0.001, file name='layer', early stopp=True, epochs=1000,
                        root dir=os.path.join(os.getcwd(), "export data\DNN model save"),):
              model.compile(optimizer=tf.keras.optimizers.Adam(learning rate=lr 0, ), \#decay=0.01, lr=lr 0/(1+decay*iteration)
                            loss='sparse_categorical_crossentropy', metrics=['accuracy'], steps_per_execution=10)
              run id = time.strftime("%Y %m %d %H %M %S ")
              log dir = os.path.join(root dir, run id+file name+' lr'+str(lr 0))
              output model file = os.path.join(log dir, 'best model.h5')
              checkpoint cb = tf.keras.callbacks.ModelCheckpoint(filepath=output model file, save best only=<math>true) #save only when best t
              tensorboard callback = tf.keras.callbacks.TensorBoard(log dir=log dir, histogram freq=2) # Enable histogram computation wi
              if early stopp == True:
                  early stopping cb = tf.keras.callbacks.EarlyStopping(patience=50, min delta=1e-4, restore best weights=True) #roll back
                  callbacks=[tensorboard callback, checkpoint cb, early stopping cb]
              elif early stopp == False:
                  callbacks=[tensorboard callback, checkpoint cb]
              df train x, df train y, df test x, df test y = split train test(data mov, y col='type num', split y=True)
              history = model.fit(x=df_train_x, y=df_train_y,
                                  epochs=epochs, verbose=1,
                                  validation data=(df test x, df test y),
                                  callbacks=callbacks)
              return history
          data_mov = moving_avg(df_import['size+imp+3Ab'], n=10, skip='PS', random_state=42)#5imp
In [790...
          data mov['type num'] = [type 2 num[i] for i in data mov['type']]
          temp = data_mov.loc[:,['type_num','type']].copy(deep=True)
          df drop = data mov.drop(columns=['type num','type'])
          df normalized = MinMaxScaler((0,1)).fit transform(df drop)
          df processed = pd.DataFrame(df normalized, columns=df drop.columns, index=df drop.index)
```

```
df avg norm = pd.concat([df processed, temp], axis=1)
          df train x, df train y, df test x, df test y = split train test(data mov, y col='type num', split y=True)
 In [8]: model = create model(input shape=(5), output=4, Dense=[30,10,5])
          root dir=os.path.join(os.getcwd(), "export data\DNN model save")
          run id = time.strftime("%Y %m %d %H %M %S")
          history = run model(model , df avg norm, lr 0=0.001, file name='size+imp+3Ab layer5 30 10 5',
                               early stopp=False, root dir=root dir, epochs=1000)
          train hist = pd.DataFrame(history .history)
          train hist .to excel(os.path.join(root dir, run id+'size+imp+3Ab layer5 30 10 5 lr0.001.xlsx'))
In [854...] fig, ax1 = plt.subplots(figsize=(4,3), dpi=150)
          cmap=sns.diverging palette(240, 10, s=80, l=60, sep=20, n=4)
          ax1.set xlabel('epoch')
          te a, = ax1.plot(train hist .index, train hist ['val accuracy'], color=cmap[1], label='test accuracy')
          tr a, = ax1.plot(train hist .index, train hist ['accuracy'], color=cmap[0], label='training accuracy')
          ax1.set ylabel('Accuracy')
          ax1.set_ylim([0.1,1.05])
          ax1.spines["left"].set color(cmap[0])
          ax2 = ax1.twinx()
          te 1, = ax2.plot(train hist .index, train hist ['val loss'], color=cmap[2], label='test loss')
          tr 1, = ax2.plot(train hist .index, train hist ['loss'], color=cmap[3], label='training loss')
          ax2.set ylabel('Loss')
          #ax2.set_ylim([0,1.6])
          ax2.spines["right"].set color(cmap[3])
          ax2.spines["left"].set visible(False)
          plt.legend(handles=[tr a, te a, tr l, te l], loc='center right', fontsize=8)
```

Out[854... <matplotlib.legend.Legend at 0x1f408bf1b50>



Note: training: average of each epoch; test: on the end of each epoch

run_func

```
run history = {}
for key in data dict:
    history n = []
    for n in n range:
        data mov = moving avg(data dict[key], n=n, skip=skip mov, random state=random state)
        data_mov['type_num'] = [type_2_num[i] for i in data_mov['type']]
        if key != skip norm:
            temp = data mov.loc[:,['type num','type']].copy(deep=True)
            df drop = data mov.drop(columns=['type num','type'])
            df normalized = MinMaxScaler((0,1)).fit transform(df drop)
            df processed = pd.DataFrame(df normalized, columns=df drop.columns, index=df drop.index)
            df avg norm = pd.concat([df processed, temp], axis=1)
        else:
            df avg norm = data mov.copy(deep=True)
        model = create_model(input_shape=df_avg_norm.shape[1]-2, output=len(df_avg_norm['type'].unique()), Dense=Dense)
        history = run model(model, df avg norm, lr 0=lr 0, file name=key+' n='+str(n),
                            early stopp=early stopp, root dir=root dir)
        history_n += [history]
        accu train.loc[n, key] = history.history['accuracy'][-1]
        accu_test.loc[n, key] = history.history['val_accuracy'][-1]
        loss train.loc[n, key] = history.history['loss'][-1]
        loss test.loc[n, key] = history.history['val loss'][-1]
    run history[key] = history n
return accu train, accu test, loss train, loss test, run history
```