Sorting Mock Galaxy Observations with Unsupervised Methods

Bobby Bickley, Phys. 555 2020

I will be using CNN-autoencoder dimensionality reduction, kmeans clustering, and t-SNE dimensionality reduction in series to explore 40,000 mock observations of galaxies, though the data set in this graphical version is about 1/10 that size, for visualization purposes. The images were constructed by convolving Illustris-TNG galaxies with a custom observational realism suite, RealSimCFIS, so that they appear as they might if observed by the Canada-France Imaging Survey (CFIS), hosted by CFHT on Mauna Kea, Hawaii. CFIS images have a formidable level of detail, but due to inevitable observational errors, gaps in the survey, and erroneous celestial objects, they are sometimes affected by survey "artifacts", here meaning any one of a list of several atypical image features that result in difficulty in analyzing an image. For the sake of realism, these artifacts are included in the data set. However, situations may arise wherein it is helpful to increase the purity of the sample by limiting the number of included features. It is also a productive exercise to develop an architecture that separates artifacts in a RealSimCFIS capacity; one could develop an artifact separation pipeline on the mock survey's many images that could later be applied to real CFIS data.

```
In [1]: #Imports
        from six.moves import urllib
        from sklearn.decomposition import PCA
        from scipy.io import loadmat
        from matplotlib import pyplot
        from sklearn.metrics import confusion_matrix
        import itertools
        from sklearn import preprocessing
        import keras
        from IPython.display import clear_output
        from sklearn.linear model import LogisticRegression
        from keras.layers import Input, Dense
        from keras.models import Model
        import itertools
        import numpy as np
        import matplotlib.pyplot as plt
        from astropy.io import fits
        import tarfile
        from keras.layers import Input, Dense, Conv2D, MaxPooling2D, UpSampling2D, Flatten
        from keras.models import Model
        from keras import backend as K
        import os, sys
        from sklearn import svm, datasets
        from sklearn.model selection import train test split
        import cv2
        from skimage.transform import resize
        from sklearn.cluster import KMeans
        from sklearn.manifold import TSNE
        Using TensorFlow backend.
        /Users/robertbickley/anaconda3/lib/python3.7/site-packages/tensorflow/python/frame
        work/dtypes.py:516: FutureWarning: Passing (type, 1) or 'ltype' as a synonym of ty
        pe is deprecated; in a future version of numpy, it will be understood as (type,
        (1,)) / '(1,)type'.
          _np_qint8 = np.dtype([("qint8", np.int8, 1)])
        /Users/robertbickley/anaconda3/lib/python3.7/site-packages/tensorflow/python/frame
        work/dtypes.py:517: FutureWarning: Passing (type, 1) or 'ltype' as a synonym of ty
        pe is deprecated; in a future version of numpy, it will be understood as (type,
        (1,)) / '(1,)type'.
          np quint8 = np.dtype([("quint8", np.uint8, 1)])
        /Users/robertbickley/anaconda3/lib/python3.7/site-packages/tensorflow/python/frame
        work/dtypes.py:518: FutureWarning: Passing (type, 1) or 'ltype' as a synonym of ty
        pe is deprecated; in a future version of numpy, it will be understood as (type,
        (1,)) / '(1,)type'.
          np qint16 = np.dtype([("qint16", np.int16, 1)])
        /Users/robertbickley/anaconda3/lib/python3.7/site-packages/tensorflow/python/frame
        work/dtypes.py:519: FutureWarning: Passing (type, 1) or 'ltype' as a synonym of ty
        pe is deprecated; in a future version of numpy, it will be understood as (type,
        (1,)) / '(1,)type'.
          _np_quint16 = np.dtype([("quint16", np.uint16, 1)])
        /Users/robertbickley/anaconda3/lib/python3.7/site-packages/tensorflow/python/frame
        work/dtypes.py:520: FutureWarning: Passing (type, 1) or 'ltype' as a synonym of ty
        pe is deprecated; in a future version of numpy, it will be understood as (type,
        (1,)) / '(1,)type'.
          np qint32 = np.dtype([("qint32", np.int32, 1)])
        /Users/robertbickley/anaconda3/lib/python3.7/site-packages/tensorflow/python/frame
        work/dtypes.py:525: FutureWarning: Passing (type, 1) or 'ltype' as a synonym of ty
        pe is deprecated; in a future version of numpy, it will be understood as (type,
        (1,)) / '(1,)type'.
          np resource = np.dtype([("resource", np.ubyte, 1)])
        /Users/robertbickley/anaconda3/lib/python3.7/site-packages/tensorboard/compat/tens
        orflow stub/dtypes.py:541: FutureWarning: Passing (type, 1) or 'ltype' as a synony
        m of type is deprecated; in a future version of numpy, it will be understood as (t
```

ype, (1,)) / '(1,)type'.

nn ain+8 = nn d+vne/[("ain+8" nn in+8 1)])

The PlotLosses class was useful to visually observe the training history of various models in our course exercises, and I have reproduced it here. All credit to the instructors of PHYS555.

```
In [2]: #PlotLosses class borrowed from class exercises
        class PlotLosses(keras.callbacks.Callback):
            def on train begin(self, logs={}):
                self.i = 0
                self.x = []
                self.losses = []
                self.val losses = []
                self.fig = plt.figure()
                self.logs = []
            def on epoch end(self, epoch, logs={}):
                self.logs.append(logs)
                self.x.append(self.i)
                self.losses.append(logs.get('loss'))
                self.val losses.append(logs.get('val loss'))
                self.i += 1
                clear_output(wait=True)
                plt.plot(self.x, self.losses, label="train")
                plt.plot(self.x, self.val losses, label="validation", linestyle='--')
                plt.legend()
                plt.show();
        plot losses = PlotLosses()
```

Now for data retrieval; first defining a method open a tarball of 4 images (corresponding to one galaxy photographed at 4 angles), and extract the fits data from the specified image within the tarball.

```
In [2]: #My own function to grab data from an image file, which is a tarball of the 4 camera
def im_look(filename,cam):
    sci_tar = tarfile.open(filename)
    membs=sci_tar.getmembers()
    im_dat = fits.getdata(sci_tar.extractfile(membs[cam]))
    sci_tar.close()
    return im_dat
```

```
In [3]: #Retrieve galaxy image data from wherever it is stored on your machine
    data_dir = '/Users/robertbickley/Documents/UVic/y1/ML/project/sci_ims_1/'
    data_files = os.listdir(data_dir)
    if '.DS_Store' in data_files: data_files.remove('.DS_Store')
    data_files = [data_dir+i for i in data_files]
    inp = np.array([resize(im_look(f,c),(128,128)) for f in data_files for c in range(4))
```

Please note: to produce the figures in this notebook, I used a smaller dataset of ~4000 images, so that I could complete it in an interactive session. For the results shown in my presentation, I will be using a sample 10x larger than that, ~40,000 images, to get more robust results. Running with 40,000 images is not feasible in an interactive session, however. Here we normalize the data using a simple minmax normalization, before flattening it for our first round of tests.

```
In [4]: #normalize
    inp = [i-np.amin(i) for i in inp]
    inp = [i/np.amax(i) for i in inp]
    inp_flat = np.reshape(inp,(-1,16384))
```

```
In [6]: #Visualize thumbnails of a few of the galaxies
n = 8  # how many galaxies we will display
plt.figure(figsize=(20, 4))
for i in range(n):
    ax = plt.subplot(2, n, i + 1)
    plt.imshow(np.log10(np.reshape(inp_flat[i],(128,128))))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)
```

/Users/robertbickley/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py: 6: RuntimeWarning: divide by zero encountered in log10

















Autoencoder

Here we define and test our first autoencoder, which only uses dense layers. An autoencoder will be helpful here, because we will be able to reduce the effective size of the individual images in subsequent steps, aiding in our fight against dimensionality. The primary issue with a dense-only autoencoder is that spatial information in the original data is mostly not preserved, but it is nonetheless interesting to check what information the network is able to retain.

```
In [5]: #Split the data
inp_tr,inp_va = train_test_split(inp_flat,test_size=.2,random_state=0)
```

```
In [8]: #Define a deep, under-complete autoencoder with only dense layers
        encoding dim = 128
        # this is our input placeholder
        input img = Input(shape=(16384,))
        encoded = Dense(2048, activation='relu')(input_img)
        encoded = Dense(512, activation='relu')(encoded)
        z = Dense(encoding_dim, activation='relu', name = 'latent_layer')(encoded)
        z= keras.layers.BatchNormalization()(z)
        decoded = Dense(512, activation='relu')(z)
        decoded = Dense(2048, activation='relu')(decoded)
        decoded = Dense(16384, activation='sigmoid')(decoded)
        # this model maps an input to its encoded representation
        encoder = Model(input img, z)
        # this model maps an input to its reconstruction
        autoencoder = Model(input_img, decoded)
        autoencoder.summary()
```

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:74: The name tf.get_default_graph is deprecat ed. Please use tf.compat.v1.get_default_graph instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:517: The name tf.placeholder is deprecated. P lease use tf.compat.v1.placeholder instead.

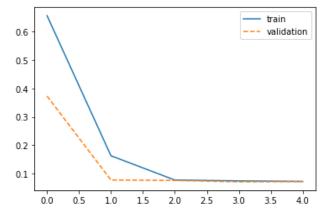
WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:4138: The name tf.random_uniform is deprecate d. Please use tf.random.uniform instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:133: The name tf.placeholder_with_default is deprecated. Please use tf.compat.v1.placeholder with default instead.

Layer (type)	Output	Shape	Param #
<pre>input_1 (InputLayer)</pre>	(None,	16384)	0
dense_1 (Dense)	(None,	2048)	33556480
dense_2 (Dense)	(None,	512)	1049088
latent_layer (Dense)	(None,	128)	65664
batch_normalization_1 (Batch	(None,	128)	512
dense_3 (Dense)	(None,	512)	66048
dense_4 (Dense)	(None,	2048)	1050624
dense_5 (Dense)	(None,	16384)	33570816
Total params: 69,359,232 Trainable params: 69,358,976 Non-trainable params: 256	=====		

A standard training loop. In many tests, this network was trained for up to 100 epochs, though the performance largely does not improve. In the thumbnails below, you can see that only the presence of a central bright object is preserved in the reconstructed images.

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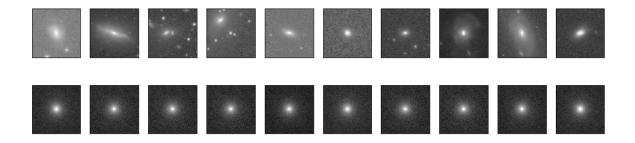
Out[9]: <keras.callbacks.History at 0x1c50a81ed0>

```
In [10]: #Make dense encoder predictions on the data
    decoded_tr = autoencoder.predict(inp_tr)
    decoded_va = autoencoder.predict(inp_va)
    print('The size of the latent validation set == ', np.shape(decoded_va))
```

The size of the latent validation set == (788, 16384)

```
In [11]: n = 10  # how many galaxies we will display
plt.figure(figsize=(16,4))
for i in range(n):
    # display original
    ax = plt.subplot(2, n, i + 1)
    plt.imshow(np.log10(inp_va[i].reshape(128, 128)))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)
    # display reconstruction
    ax = plt.subplot(2, n, i + 1 + n)
    plt.imshow(np.log10(decoded_va[i].reshape(128, 128)))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)
    plt.show()
```

/Users/robertbickley/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py: 6: RuntimeWarning: divide by zero encountered in log10



CNNs were developed specifically for their ability to retain and learn from spatial information in images. Here we define a similarly-constructed autoencoder, except using Conv2D and MaxPooling layers in our encoder, and Conv2D and UpSampling2D in our decoder. Because this autoencoder will be the one that we use in subsequent steps, we also save the encoder separately, as it will be used, as the name implies, to encode our data.

```
In [6]: #With the limited success of a dense-only autoencoder, let's try a CNN autoencoder
        #Autoencoder CNN
        input_img = Input(shape=(128, 128, 1)) # adapt this if using `channels_first` image
        x = Conv2D(16, (3, 3), activation='relu', padding='same')(input_img)
        x = MaxPooling2D((2, 2), padding='same')(x)
        x = Conv2D(8, (3, 3), activation='relu', padding='same')(x)
        x = MaxPooling2D((2, 2), padding='same')(x)
        x = Conv2D(4, (3, 3), activation='relu', padding='same')(x)
        z = MaxPooling2D((2, 2), padding='same', name='latent_layer')(x)
        z= keras.layers.BatchNormalization()(z)
        x = Conv2D(4, (3, 3), activation='relu', padding='same')(z)
        x = UpSampling2D((2, 2))(x)
        x = Conv2D(8, (3, 3), activation='relu', padding='same')(x)
        x = UpSampling2D((2, 2))(x)
        x = Conv2D(16, (3, 3), activation='relu', padding='same')(x)
        x = UpSampling2D((2, 2))(x)
        x = Conv2D(16, (3, 3), activation='sigmoid', padding='same')(x)
        decoded = Conv2D(1, (3, 3), activation='sigmoid', padding='same')(x)
        autoencoder = Model(input_img, decoded)
        autoencoder.compile(optimizer='adadelta', loss='binary_crossentropy')
        # this model maps an input to its encoded representation
        encoder = Model(input img, z)
        # this model maps an input to its reconstruction
        autoencoder = Model(input img, decoded)
        autoencoder.summary()
```

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:74: The name tf.get_default_graph is deprecat ed. Please use tf.compat.v1.get_default_graph instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:517: The name tf.placeholder is deprecated. P lease use tf.compat.v1.placeholder instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:4138: The name tf.random_uniform is deprecate d. Please use tf.random.uniform instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:3976: The name tf.nn.max_pool is deprecated. Please use tf.nn.max_pool2d instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:174: The name tf.get_default_session is depre cated. Please use tf.compat.v1.get_default_session instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:181: The name tf.ConfigProto is deprecated. P lease use tf.compat.v1.ConfigProto instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:1834: The name tf.nn.fused_batch_norm is deprecated. Please use tf.compat.v1.nn.fused batch norm instead.

WARNING:tensorflow:From /Users/robertbickley/anaconda3/lib/python3.7/site-packages /keras/backend/tensorflow_backend.py:2018: The name tf.image.resize_nearest_neighb or is deprecated. Please use tf.compat.v1.image.resize_nearest_neighbor instead.

WARNING.tensorflow.From /Hsers/roberthickley/anaconda3/lih/nython3 7/site_nackages

```
In [7]: #Since we will be using the CNN autoencoder for our next steps, we define an encoder
encoder = Model(input_img,z)
encoder.summary()
```

Layer (type)	Output Shape	Param #
input_1 (InputLayer)	(None, 128, 128, 1)	0
conv2d_1 (Conv2D)	(None, 128, 128, 16)	160
max_pooling2d_1 (MaxPooling2	(None, 64, 64, 16)	0
conv2d_2 (Conv2D)	(None, 64, 64, 8)	1160
max_pooling2d_2 (MaxPooling2	(None, 32, 32, 8)	0
conv2d_3 (Conv2D)	(None, 32, 32, 4)	292
latent_layer (MaxPooling2D)	(None, 16, 16, 4)	0
batch_normalization_1 (Batch	(None, 16, 16, 4)	16
Total params: 1,628 Trainable params: 1,620 Non-trainable params: 8		

```
In [8]: #Because this model takes 2D input, we un-reshape our data back to its original size
inp_tr2D = np.reshape(inp_tr, (len(inp_tr), 128, 128, 1))
inp_va2D = np.reshape(inp_va, (len(inp_va), 128, 128, 1))
```

Here, the training loop is effectively the same as for our last autoencoder. Because this step may be time consuming, I've commented out the training loop, and simply load the weights from a file I prepared. For a given data set, however, retraining is absolutely necessary.

```
In [9]: #Training code is commented out because the model was trained in an earlier session.
# autoencoder.compile(optimizer='adadelta', loss='binary_crossentropy')
# autoencoder.fit(inp_tr2D, inp_tr2D,
# epochs=100,
# batch_size=128,
# shuffle=True,
# validation_data=(inp_va2D, inp_va2D), callbacks=[plot_losses])
# autoencoder.save_weights('autoenc_model.h5')

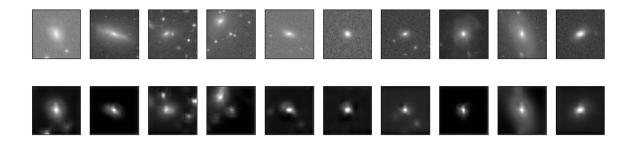
#Instead, we load the saved weights from a file
autoencoder.load_weights('autoenc_model.h5')
```

Now we use our updated autoencoder to make predictions about our data set, effectively collapsing the data to a much smaller size for the next step, Kmeans clustering.

```
In [11]: #Make CNN encoder predictions on the data
decoded_tr = autoencoder.predict(inp_tr2D)
decoded_va = autoencoder.predict(inp_va2D)
print('The size of the latent validation set == ', np.shape(decoded_va))
The size of the latent validation set == (788, 128, 128, 1)
```

```
In [12]: n = 10 # how many galaxies we will display
         plt.figure(figsize=(16,4))
         for i in range(n):
             # display original
             ax = plt.subplot(2, n, i + 1)
             plt.imshow(np.log10(inp_va[i].reshape(128, 128)))
             plt.gray()
             ax.get xaxis().set visible(False)
             ax.get yaxis().set visible(False)
             # display reconstruction
             ax = plt.subplot(2, n, i + 1 + n)
             plt.imshow(np.log10(decoded va[i].reshape(128, 128)))
             plt.gray()
             ax.get xaxis().set visible(False)
             ax.get yaxis().set visible(False)
         plt.show()
```

/Users/robertbickley/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py: 6: RuntimeWarning: divide by zero encountered in log10



The effects of this encoder are much more suitable; erroneous background objects and noise are largely ignored, while the size, rough shape, and positions of primary bright objects in each image are preserved, albeit with some artifacts.

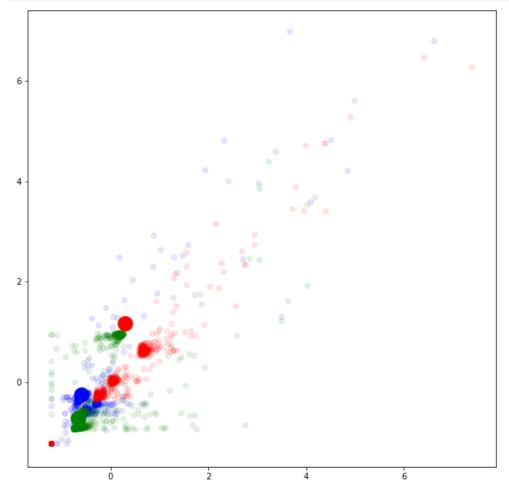
```
In [16]: #Make predictions using the new encoder
encoded_va = encoder.predict(inp_va2D)
encoded_tr = encoder.predict(inp_tr2D)
```

Kmeans

Now, with the dimensionality of our input data reduced by about an order of magnitude, we set about the test of clustering the data. Kmeans has proven to be very effective in doing this, and in separating artifacts from "normal" images, as you will see with examples plotted below. The Kmeans algorithm iteratively explores data in arbitrarily-high dimensional space, searching for the separations that optimize a loss function with a user-specified number of clusters.

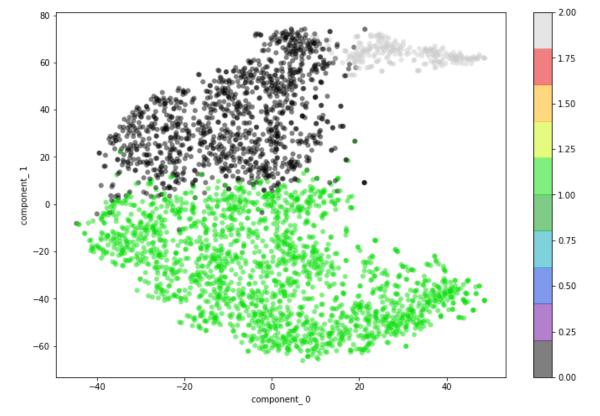
```
In [17]: #Now, we will feed the encoded data into a Kmeans algorithm, first with K=3, as an e
K = 3
#Change the reshape statement to reflect the sizes of your training and testing set
kmeans = KMeans(n_clusters=K).fit(encoded_tr.reshape(3152,-1))
Kmean_tr=kmeans.predict(encoded_tr.reshape(3152,-1))
Kmean_va=kmeans.predict(encoded_va.reshape(788,-1))
```

Now that we have made predictions, we will attempt to visualize the work that Kmeans have done in high-dimensional clustering. This is non-trivial, however; choosing two dimensions at random upon which to project the data is not an optimal way to visualize the data, as you will see.



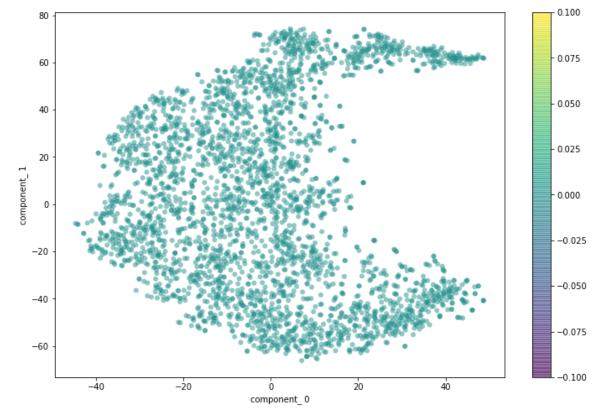
Because this visualization is not especially productive, let's use t-SNE to collapse the >1000-D data into two dimensions, and re-plot it. This should give us some insight into how well our clustering has worked.

```
In [20]: #Make a plot of the T-SNE result
    #t-SNE plot
    comp_x=0
    comp_y=1
    plt.figure(figsize=(12,8))
    plt.scatter(tsne_results_tr[:,comp_x], tsne_results_tr[:,comp_y], edgecolor='none',
    plt.xlabel('component_ '+ str(comp_x))
    plt.ylabel('component_ '+str(comp_y))
    plt.colorbar()
    plt.show()
```



Kmeans allows for differential population sizes within clusters, which is critical to this project. You can see that cluster 2 (gray) is significantly smaller than the other two. Visually though, how do the members of cluster 3 differ? And further, how do they corellate to naive algorithmic measures of "artifacts", such as zero-flux pixel fraction? We explore these questions in the following plots.

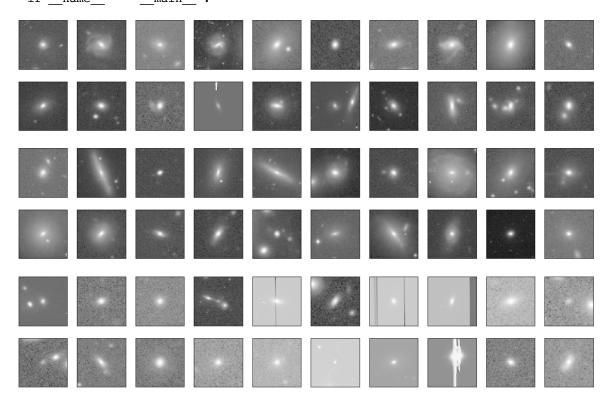
```
In [21]: #How do we compare to our naively-defined artifact metric, the zero-flux-pixel fract
#Take naive "artifact" statistic of f_zer, and split them into the same two sets as
f_zers = [len(np.argwhere(im>1))/(len(im)**2) for im in inp]
fr_tr,fr_va = train_test_split(f_zers,test_size=.2,random_state=0)
#alt t-SNE plot to show separation of naively-defined artifacts
plt.figure(figsize=(12,8))
plt.scatter(tsne_results_tr[:,comp_x], tsne_results_tr[:,comp_y], edgecolor='none',
plt.xlabel('component_ '+ str(comp_x))
plt.ylabel('component_ '+str(comp_y))
plt.colorbar()
plt.show()
```



Our naive zero-flux pixel fraction metric doesn't help too much here, though a detailed investigation reveals that the few images with significant zero-flux pixel fractions fall into category 2, at the tip of the t-SNE collapsed distribution. In our thumbnails below, we find that category 2, in the bottom two rows, collects many, though certainly not all, of the image-dominated artifacts. It also, however, captures many galaxies that were observed with good quality.

```
In [22]: #Let's inspect images that were placed into each of the three classes
for n in range(3):
    fig, axs = plt.subplots(2,10,figsize=(20, 4))
    count = 0
    #Plotting 2x10 images for each Kmean cluster
    for i in range(2):
        for j in range(10):
            plt.gray()
            axs[i][j].imshow(np.log10(np.reshape(inp_tr[Kmean_tr==n][count],(128,128 axs[i][j].get_xaxis().set_visible(False)
            axs[i][j].get_yaxis().set_visible(False)
            count +=1
    plt.show()
```

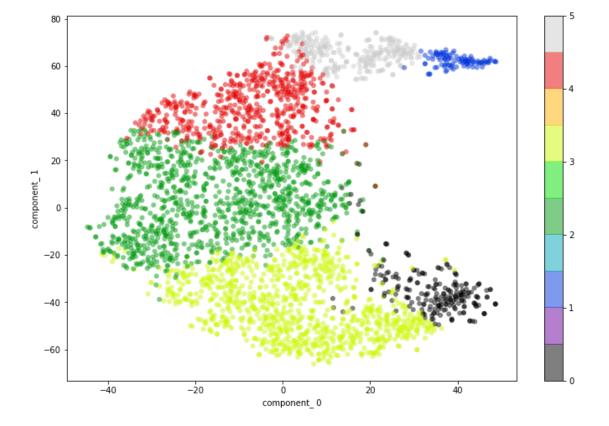
/Users/robertbickley/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:
9: RuntimeWarning: divide by zero encountered in log10
 if name == ' main__':



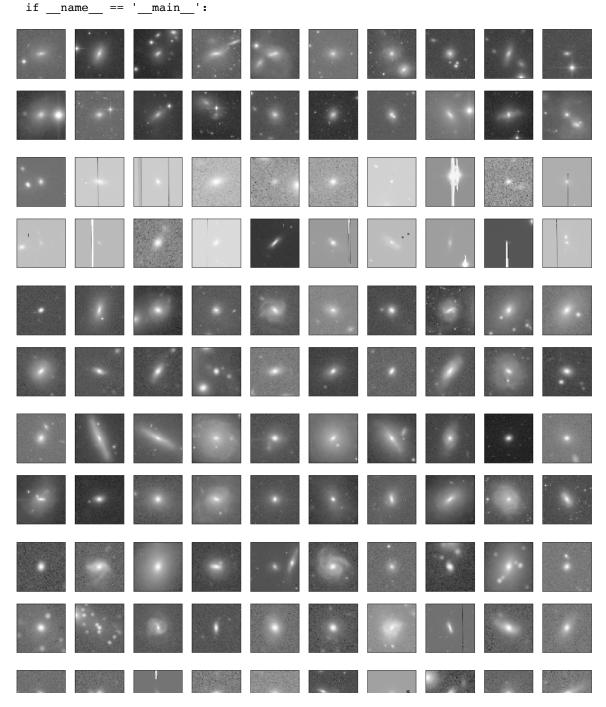
With K = 3, the third category (last two rows above) captures the visible artifacts, though with a coarse brush. A larger number of "normal" images are also included.

```
In [23]: #Now, we'll repeat the last few steps with our final K-value, 6
K=6
# fit the n first components of pca by Kmean
kmeans = KMeans(n_clusters=K).fit(encoded_tr.reshape(3152,-1))
Kmean_tr=kmeans.predict(encoded_tr.reshape(3152,-1))
Kmean_va=kmeans.predict(encoded_va.reshape(788,-1))
```

Out[24]: <matplotlib.colorbar.Colorbar at 0x1c6657d710>



/Users/robertbickley/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:
9: RuntimeWarning: divide by zero encountered in log10



With K = 6, there is a small tradeoff, but with net positive results. While a few, less-catastrophic artifact images are included in other categories, the second category (rows 3 and 4 in the image above) contains a much higher density of artifact images than with other categories. Repeating this, as I will show in my presentation, with K=7, yields another interesting result - that you can specify two artifact clusters. They capture nearly all of the artifacts, allowing for extreme purity in the rest of the clusters.

In []:	:	