```
import pandas as pd
import numpy as np
import keras
from keras import layers
# May need to import more things (e.g regularizers)
```

Upload the labels.csv and processed\_counts.csv files to colab or your local workspace.

This data associates a cell barcode, such as "AAAGCCTGGCTAAC-1", to a certain cell type label, such as "CD14+ Monocyte". For each cell barcode, there are also log RNA seq counts of 765 different genes, such as HES4.

label.csv stores the association between a cell barcode and a cell type label.

processed\_counts.csv stores the normalized log read counts for each cell, where each row represents a single cell, and each column represents a gene.

```
labels_pd = pd.read_csv("labels.csv")
counts_pd = pd.read_csv("processed_counts.csv")
labels_pd

counts_pd.rename(columns = {'Unnamed: 0':'index'}, inplace = True)
counts_pd
```

```
HES4 TNFRSF4 SSU72 PARK7
                                                             RBP7
                                                                     SRM MAD2L2 AGTRAP
                       index
           AAAGCCTGGCTAAC-
      0
                              -0.326
                                       -0.191
                                              -0.728 -0.301
                                                             3.386 -0.531
                                                                            2.016
                                                                                    3.377
counts pd
labels pd
labeled_counts = pd.merge(counts_pd, labels_pd, on="index")
           -0.326
                                       -0.191
                                               1.134 -0.157 -0.174 -0.531
                                                                           -0.451
                                                                                   -0.486
labeled counts
                                       -0.191 -0.728 -0.607 -0.174 -0.531
                             -0.326
                                                                           -0.451
                                                                                    0.787
Shuffle your data. Make sure your labels and the counts are shuffled together.
Split into train and test sets (80:20 split)
# https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.ShuffleSpl
from sklearn.model_selection import ShuffleSplit
#counts_pd
#labels pd
X = \text{np.array}([[1, 2], [3, 4], [5, 6], [7, 8], [3, 4], [5, 6]])
y = np.array([1, 2, 1, 2, 1, 2])
rs = ShuffleSplit(n_splits=1, test_size=.20, random state=0)
rs.get n splits(counts pd)
for train_index, test_index in rs.split(counts_pd,labels_pd):
  print("TRAIN:", train index, "TEST:", test index)
  print(train index.shape)
  print(test index.shape)
  break
```

```
TRAIN: [ 45 285 62 386 668 299 140 584 490 127 665 144
                                                         21 480 511
  77 249 333 374 263 101 279 196 294 170 460 542 409 477 691 696 214 165
     34 685 200 596 155 316 215 547 451 494
                                              12 161 690 561 443 258 159
 338
     78
         92 476 66 261 319 283 641 271 369 540 623
                                                      15 420 247
 71 517 408 315 303 104 632 188 395 351 404 686
                                                  90 603 245 204 350 118
 293 661 218 519 250 616 415 109 375 205 339 190 327 681 439 390 495 647
 479 194 362 452 310 422 332 132 233 173 178 678 530 206
                                                          96 601 571 385
                46 171 558 570 107 505 392 223 397 102 108 213 426 649
 89 355 179
               0
 246 416 367 125 608 498 478 566 224
                                      26 403 484 497
                                                       3 134 317 186 516
 295 585 552 631 225 573 568 500 458 669 434 622 342 527 112 482
                                                                   20
                                                                       65
 298 126 259 521 440 586 137 436
                                   7 643 309 474 185 402 153
                                                              54
                                                                   30 625
```

```
100 652 576 664 237
                      56
                          60 496 262 535 264 653 400 208 453 391 167
609 572 300 441 432 682 163 124 154 336
                                           59 642 304 657 549 343 526 311
          51 499 462 567 361 399 425 219 308
                                               74 282 449
                                                             4 597 541 424
             513 135
                    447
                         378
                             628
                                   22 636
                                          276 284
                                                  270 670 281
                                                               220 634
483 120
                     419
                         679 672 160 699 238 379 579 485 492 523 195 191
116 534 602 164 106
                      16
                          63 384 105 489 660 329
                                                  345 612 405 522
     83 591 348 648 198 145 414 150
                                       39 514 615 640 539 322 253 627 663
688 357
                 340
                    221 654 146
                                 289 241
                                           29 577
                                                  114 487
                                                          695
651 372 168 347 376 531 613 598 680 189 136 446
                                                  588 254
                                                          437 382 620
                              88 418 290
662 618 593 255 232 133
                                           44 353 341
                          33
                                                       61
                                                          671 199 429 394
     73 393 692 583 589 217 578 421 138 212 590 587 644 234
                                                                    24 381
297
                                                                67
216 129 349 111 166 207 438 274 595 698 525 287 469 326 121 507 228 445
117 464
          25 110 149 152 528 461 139 260 323 630 248 450 410
                                                                19 328 296
269 226
          94 515 280 286 655 444 184 371 614 683 275 658 182
                                                                32
                                                                    80 307
 11
     43
          86
              36
                  58
                      41 411 562 209 148 594 123 574
                                                       98 377 130
                                                                    23 638
555 370 512 383 201 368 554 610 387 292 256 606 197
                                                       95 676 169 581 305
560 373 227 143 180 131
                          47 324 203
                                       84 633 565 611 398
                                                            91
                                                                82 430 119
      57 321 257 666 442
                          42 617 388 335 273 488 550
                                                       53 673 128
459 510 151 244 543 544 639 265 288 423 147 659 177
                                                       99
                                                          448 431 115
537 677 689 174
                  87 551 486 314 396 600 472
                                               70 599 277
                                                             9 359 192 629
559 684] TEST: [306 604
                          40 493
                                   14 548 267
                                               31 252 103 675
                                                              278
                                                                  536 313
                                                                            85 352
529 502 545 344 624 621 582 538 520 533 619
                                                1 546 235 172
407 468 231 229 181
                      27 210 401 364 465 471 569 463 592 356 646 366 637
406 312 360 142
                   8
                      79 365 175 193 354
                                           50 656 491 607 455 605 330
                                                                        10
 68 467 694 239 473 524 230 575 650 358 318 268 635
                                                      457 122 302 251 626
157 693 389 346
                  37 243
                          48 481 454 240 162 508
                                                   76
                                                       64
                                                            52 557 334 236
                                                           97
674 563 428 187 331 156 363 325 222 435 456 470 113 697
                                                                18 506 301
     49 380 466 211
                      17 503 202 580 337 266 645 504 4171
(560,)
140,)
```

Create a fully connected neural network for your autoencoder. Your latent space can be of any size less than or equal to 64. Too large may result in a poor visualization, and too small may result in high loss. 32 is a good starting point.

Consider using more than 1 hidden layer, and a sparcity constraint (I1 regularization).

Have an encoder model which is a model of only the layers for the encoding.

```
#discussion model
import keras
from keras import layers
from keras import regularizers
import tensorflow as tf

encoding_dim = 32 # 32 floats (we're going from 767 dimensions -> 32 dimensions)
input_img = keras.Input(shape=(765,))

### OG
#encoded = layers.Dense(encoding_dim, activation='relu',activity_regularizer=regulari:
#decoded = layers.Dense(765, activation='sigmoid')(encoded)
```

### OG

```
### new
encoded = layers.Dense(128, activation='relu', activity regularizer=regularizers.l1(10)
#encoded = layers.Dense(64, activation='relu', activity_regularizer=regularizers.l1(10)
encoded = layers.Dense(32, activation='relu', activity_regularizer=regularizers.11(10@
decoded = layers.Dense(32, activation='relu')(encoded)
#decoded = layers.Dense(128, activation='relu')(decoded)
decoded = layers.Dense(765, activation='sigmoid')(decoded)
##### new
autoencoder = keras.Model(input img, decoded)
encoder = keras.Model(input img, encoded)
autoencoder.compile(optimizer='adam', loss=tf.keras.losses.MeanSquaredError())
train index = train index.tolist()
test index = test index.tolist()
counts_pd_train = counts_pd.loc[train index]
counts pd test = counts pd.loc[test index]
labels_pd_train = labels_pd.loc[train_index]
labels pd test = labels pd.loc[test index]
counts pd train np = counts pd train.copy().to numpy()
counts pd test np = counts pd test.copy().to numpy()
counts pd train np.shape
    (560, 765)
#remove the first column
#counts pd train nl = np.delete(counts pd train np,[0],1)
#counts pd test nl = np.delete(counts pd test np,[0],1)
#cleaned up data ready to be put through the autoencoder
counts pd train nl = counts pd train np.astype('float32')#/255
counts pd test nl = counts pd test np.astype('float32')#/255
counts pd test nl.shape
    (140, 765)
```

```
autoencoder.fit(counts_pd_train_nl, counts_pd_train_nl,
          epochs=5, #if redone train for just 20-30
          batch_size=256,
          shuffle=True,
          validation data=(counts pd test nl, counts pd test nl))
   Epoch 1/5
   Epoch 2/5
   Epoch 3/5
   Epoch 4/5
   Epoch 5/5
   3/3 [============= ] - 0s 56ms/step - loss: 0.9823 - val_loss: 0
   <keras.callbacks.History at 0x7ff7f08dd310>
#labels pd test['bulk labels']
counts_pd_test_nl.shape
   (140, 765)
#run on the test data
test loss = autoencoder.evaluate(counts pd test nl, counts pd test nl, verbose=2)
print('\nTest loss:', test loss)
   5/5 - 0s - loss: 0.9713 - 34ms/epoch - 7ms/step
   Test loss: 0.9713215231895447
```

Train your autoencoding using MSE loss.

Finally, identify the parameters which don't overfit, and use the same model architecture and train on all of the data together.

With a latent space size of 32, aim for 0.9 MSE loss on your test set, 0.95 with regularization. You will not be graded strictly on a loss cutoff.

#once didnt overfit, combine training and test, same autoenchoder just all the data

Use PCA and t-SNE on the dataset.

Then use PCA on the latent space representation of the dataset.

Plot all of these.

```
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
#counts pd = counts pd.drop(columns=['index'])
numpy counts = counts pd.to numpy()
# See HW7 (part 1)
#PCA on the dataset
pca = PCA(n_components=2)
counts pca = pca.fit_transform(numpy counts)
plt.figure(figsize=(10,10))
sns.scatterplot(
    x=counts_pca[:,0], y=counts_pca[:,1],
    hue=labels pd['bulk labels'],
    alpha=0.75)
plt.show()
```

```
# Carry out t-SNE on X
tsne = TSNE(n_components=2)
counts_tsne = tsne.fit_transform(numpy_counts)

/usr/local/lib/python3.7/dist-packages/sklearn/manifold/_t_sne.py:783: FutureWarn
FutureWarning,
/usr/local/lib/python3.7/dist-packages/sklearn/manifold/_t_sne.py:793: FutureWarn
FutureWarning,

plt.figure(figsize=(10,10))

sns.scatterplot(
    x=counts_tsne[:,0], y=counts_tsne[:,1],
    hue=labels_pd['bulk_labels'],
    alpha=0.75)

plt.show()
```

Compare the results of PCA, t-SNE, and your autoencoder as ways to visualize the data.

```
# Use Model.predict() to retrieve the embedding
# Use PCA on embedding
# Use tsne on embedding
### Get from encoder --> goes down to 32 dimensions
encoded counts = encoder.predict(numpy counts)
#PCA on the encoded output
pca = PCA(n components=2)
en_counts_pca = pca.fit_transform(encoded_counts)
#tsne on the encoded output
tsne = TSNE(n components=2)
en counts tsne = tsne.fit transform(encoded counts)
    /usr/local/lib/python3.7/dist-packages/sklearn/manifold/ t sne.py:783: FutureWar
      FutureWarning,
    /usr/local/lib/python3.7/dist-packages/sklearn/manifold/ t sne.py:793: FutureWar
      FutureWarning,
#encoded counts.shape
en counts pca.shape
    (700, 2)
plt.figure(figsize=(10,10))
sns.scatterplot(
    x=en_counts_pca[:,0], y=en_counts_pca[:,1],
    hue=labels pd['bulk labels'],
    alpha=0.75)
plt.show()
```

```
#prep all the data
counts np = counts pd.copy().to numpy()
counts pd t = counts np.astype('float32')
#train on entire dataset
autoencoder.fit(counts_pd_t, counts_pd_t,
             epochs=25, #if redone train for just 20-30
             batch size=256,
             shuffle=True)
   Epoch 1/25
    3/3 [=============== ] - 1s 9ms/step - loss: 1.2615
   Epoch 2/25
    3/3 [=========== ] - 0s 8ms/step - loss: 1.2537
   Epoch 3/25
    3/3 [=========== ] - 0s 8ms/step - loss: 1.2447
   Epoch 4/25
    3/3 [============= ] - 0s 8ms/step - loss: 1.2304
   Epoch 5/25
    3/3 [============= ] - 0s 9ms/step - loss: 1.2084
   Epoch 6/25
    3/3 [=========== ] - 0s 8ms/step - loss: 1.1775
   Epoch 7/25
    3/3 [=========== ] - 0s 8ms/step - loss: 1.1397
```

```
Epoch 8/25
   3/3 [============= ] - 0s 8ms/step - loss: 1.0991
   Epoch 9/25
   3/3 [============= ] - 0s 7ms/step - loss: 1.0633
   Epoch 10/25
   3/3 [============ ] - 0s 7ms/step - loss: 1.0382
   Epoch 11/25
   3/3 [========== ] - 0s 8ms/step - loss: 1.0242
   Epoch 12/25
   3/3 [============= ] - 0s 10ms/step - loss: 1.0176
   Epoch 13/25
   3/3 [============= ] - 0s 8ms/step - loss: 1.0138
   Epoch 14/25
   3/3 [============ ] - 0s 7ms/step - loss: 1.0106
   Epoch 15/25
   3/3 [============= ] - 0s 8ms/step - loss: 1.0070
   Epoch 16/25
   3/3 [============= ] - 0s 8ms/step - loss: 1.0030
   Epoch 17/25
   3/3 [============= ] - 0s 8ms/step - loss: 0.9992
   Epoch 18/25
   3/3 [============= ] - 0s 8ms/step - loss: 0.9953
   Epoch 19/25
   3/3 [============= ] - 0s 8ms/step - loss: 0.9913
   Epoch 20/25
   3/3 [============= ] - 0s 7ms/step - loss: 0.9873
   Epoch 21/25
   3/3 [============ ] - 0s 11ms/step - loss: 0.9835
   Epoch 22/25
   3/3 [============== ] - 0s 8ms/step - loss: 0.9798
   Epoch 23/25
   3/3 [=============== ] - 0s 8ms/step - loss: 0.9762
   Epoch 24/25
   3/3 [============== ] - 0s 7ms/step - loss: 0.9727
   Epoch 25/25
   3/3 [============== ] - 0s 7ms/step - loss: 0.9692
   <keras.callbacks.History at 0x7ff7f066e510>
#export the final encoded data
encoded counts final = encoder.predict(numpy counts)
df = pd.DataFrame(encoded counts final)
df.to csv('encoded counts.csv')
```



```
import pandas as pd
import numpy as np
import keras
from keras import layers
```

Upload the labels.csv and processed\_counts.csv files to colab or your local workspace.

**Copied from Part 1:** This data associates a cell barcode, such as "AAAGCCTGGCTAAC-1", to a certain cell type label, such as "CD14+ Monocyte". For each cell barcode, there are also log RNA seq counts of 765 different genes, such as HES4.

label.csv stores the association between a cell barcode and a cell type label.

processed\_counts.csv stores the normalized log read counts for each cell, where each row represents a single cell, and each column represents a gene.

```
labels_pd = pd.read_csv("labels.csv")
counts_pd = pd.read_csv("processed_counts.csv")
processed_pd = pd.read_csv("encoded_counts.csv")

df1 = processed_pd.merge(labels_pd,left_index=True, right_index=True)
df1.drop("Unnamed: 0", axis=1, inplace=True)
df1.drop("index", axis=1, inplace=True)

df1
```

0 1 2 3 4 5 6 7

**0** 0.000000 0.000000 0.000000 8.503382 0.000000 0.0 0.000000 0.0 0.000000 12.0071

```
labels_pd.index = labels_pd['index']
labels_pd.drop("index", axis=1, inplace=True)
counts_pd.index = counts_pd['Unnamed: 0']
counts_pd.drop("Unnamed: 0", axis=1, inplace=True)

df = counts_pd.merge(labels_pd, left_index=True, right_index=True).dropna()
df
```

One-hot encode the cell-type.

Shuffle your data. Make sure your labels and the counts are shuffled together.

Split into train and test sets (80:20 split)

```
#splitting up the total bulk data
categories = df['bulk labels'].unique()
print(categories)
#one-hot encoding
y = np.zeros((len(df), len(categories)))
for i in range(len(df)):
    cell type = df.iloc[i]['bulk labels']
    pos = np.where(categories == cell_type)[0]
    y[i, pos] = 1
#remove label when processing input data
X = df.drop('bulk_labels', axis=1).values
#shufle and 80:20 split
np.random.seed(100)
permutation = np.random.permutation(len(X))
X, y = X[permutation], y[permutation]
X_{train}, y_{train} = X[:int(len(X)*0.8)], y[:int(len(Y)*0.8)]
X_{\text{test}}, y_{\text{test}} = X[int(len(X)*0.8):], y[int(len(y)*0.8):]
    ['CD14+ Monocyte' 'Dendritic' 'CD56+ NK' 'CD4+/CD25 T Reg' 'CD19+ B'
      'CD8+ Cytotoxic T' 'CD4+/CD45RO+ Memory' 'CD8+/CD45RA+ Naive Cytotoxic'
      'CD4+/CD45RA+/CD25- Naive T' 'CD34+']
#splitting up the enbedded data
categories = df1['bulk labels'].unique()
print(categories)
#one-hot encoding
y = np.zeros((len(df1), len(categories)))
for i in range(len(df1)):
    cell type = df1.iloc[i]['bulk labels']
    pos = np.where(categories == cell type)[0]
    y[i, pos] = 1
#remove label when processing input data
X = df1.drop('bulk labels', axis=1).values
encoded clean = X
encoded clean labels = y
#shufle and 80:20 split
np.random.seed(100)
permutation = np.random.permutation(len(X))
X, y = X[permutation], y[permutation]
```

```
X_train1, y_train1 = X[:int(len(X)*0.8)], y[:int(len(y)*0.8)]
X_test1, y_test1 = X[int(len(X)*0.8):], y[int(len(y)*0.8):]

    ['CD14+ Monocyte' 'Dendritic' 'CD56+ NK' 'CD4+/CD25 T Reg' 'CD19+ B' 'CD8+ Cytotoxic T' 'CD4+/CD45R0+ Memory' 'CD8+/CD45RA+ Naive Cytotoxic'

#print(X_train)
#print(y_train) #one hot encoded for different cell types

print(encoded_clean.shape)
print(encoded_clean_labels.shape)

(700, 32)
    (700, 10)

#Visualize the One-hot encoded Prediction Labels
import matplotlib.pyplot as plt
plt.figure(figsize=(9,3), dpi=300)
plt.imshow(y_train[:50])
```

Apply classification algorithms to the training data, tune on validation data (if present), and evaluate on test data.

You can also apply classification downstream of last week's autoencoder latent space representation.

```
# min samples split is how many samples at each split node, (higher)
# min samples leaf is how many samples per leaf --> if low then very complex. (higher)
cross val score(clf, encoded clean, encoded clean labels, cv=5).mean()
    0.667142857142857
#random forest####
###################
#randomly pick a subset of features to work with
from sklearn.ensemble import RandomForestClassifier
#n estimators is the number of decision trees you are spitting up
#max features = 'sqrt',5 --> lower their will be less variance
#min samples split
clf = RandomForestClassifier(n_estimators=15)#, min_samples_split=2)#, max_features = 5)
clf = clf.fit(X train1,y train1)
#take average of predctions
clf.score(X test1, y test1)
    0.7071428571428572
#Ensemble bagging and random forest#
#average the predictions for multiple models
#each working with a subset of the data
from sklearn.ensemble import BaggingClassifier
#max samples is what proportion of the data is it going to train on
#max features is the max num of features each will train on
bagging = BaggingClassifier(clf, max samples=0.5, max features=0.5)
clf = clf.fit(X_train1,y_train1)
clf.score(X test1, y test1)
```

0.7357142857142858

```
# FFNN hints:
# Use softmax at the end, reLU for the rest
# Add layers until desired loss
# Categorical cross-entropy for loss func
# Add dropout layers to avoid overfitting
# Can also do bagging with FFNNs (but probably not necessary): https://machinelearning
#use all the data here
import keras
from keras import layers
from keras import regularizers
import tensorflow as tf
model = keras.Sequential()
model.add(tf.keras.Input(shape=(765)))
model.add(tf.keras.layers.Dense(100, input dim=32, activation='relu'))
model.add(tf.keras.layers.Dropout(0.3))
model.add(tf.keras.layers.Dense(100, input dim=32, activation='relu'))
model.add(tf.keras.layers.Dropout(0.3))
#model.add(tf.keras.layers.Dense(200, input dim=32, activation='relu'))
#model.add(tf.keras.layers.Dropout(0.2))
model.add(tf.keras.layers.Dense(100, input dim=32, activation='relu'))
model.add(tf.keras.layers.Dropout(0.3))
model.add(tf.keras.layers.Dense(10, activation='softmax'))
model.compile(loss="categorical crossentropy", optimizer='adam', metrics=['accuracy'])
model.fit(X_train, y_train, epochs=15)
   Epoch 1/15
   Epoch 2/15
   Epoch 3/15
   Epoch 4/15
```

```
Epoch 5/15
Epoch 6/15
Epoch 7/15
Epoch 8/15
Epoch 9/15
Epoch 10/15
Epoch 11/15
Epoch 12/15
Epoch 13/15
Epoch 14/15
Epoch 15/15
<keras.callbacks.History at 0x7fb983f67d50>
```

```
# evaluate the model

#X_train, y_train

#X_test, y_test

#0.9 achevable

_, train_acc = model.evaluate(X_train, y_train, verbose=0)

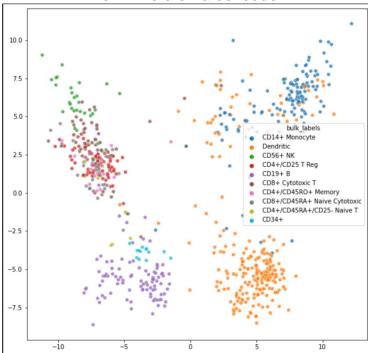
_, test_acc = model.evaluate(X_test, y_test, verbose=0)

print('Train: %.3f, Test: %.3f' % (train_acc, test_acc))
```

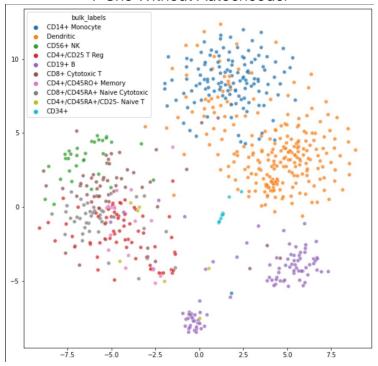
Train: 1.000, Test: 0.843

• ×

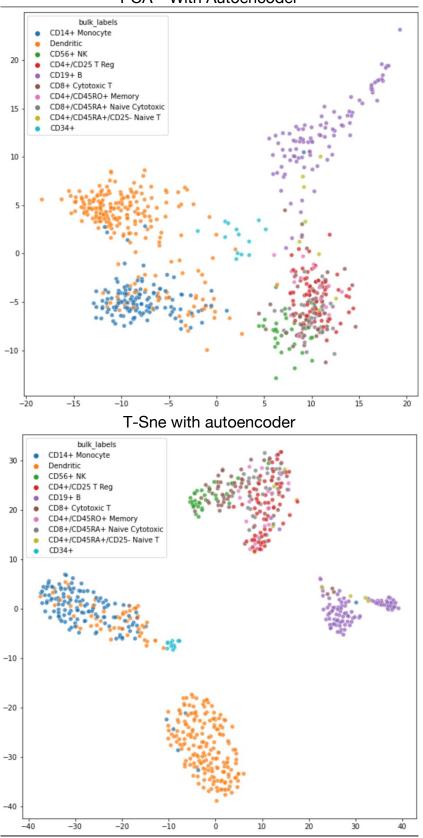
PCA - Before Autoencoder



## T-Sne Without Autoencoder

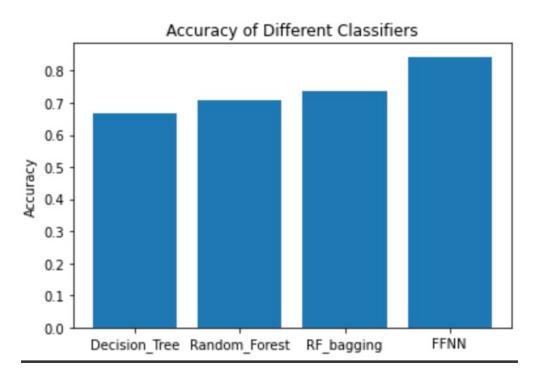


## PCA - With Autoencoder



## PART 1: Write up

The approaches I took for dimensionality reduction were PCA, T-Sne and an autoencoder. In terms of the approaches ranked from most effective to least effective I believe the autoencoder was the most effective, then the PCA then T-Sne. Looking at the autoencoder graphs in both PCA and t-Sne representations there were clearer clustering of the CD19+ B, dendritic cells and CD14+ Monocytes. Compared to the PCA and T-sne representations done before autoencoding. Looking even closer that the autoencoded data in t-sne, this graph has the clearer clustering out of all of the dimensionality reduced data. Then between the PCA and T-sne figures without autoencoding, PCA has tighter more defined clusters.



## PART 2: Write up

The four classification methods I used to try and classify the data back to cell types were a decision tree with cross-validation, random forest, random forest with bagging and finally a feed-forward neural network. The accuracy is in order from left to right is 66.7%, 70.7%, 73.6% and 84.3%. I first started with a decision tree. I found that after trial and error that the optimal parameters were a max depth of 20, with min\_samples\_split and min\_samples\_leaf at 7. Min samples split represents the number of samples at each split and min samples leaf represented the number of samples in each leaf of the tree. I kept these parameters low as I did not want the classifier to be too specific and overtrain. I also did cross validation, where I trained multiple models, 5 in my case, and take the mean of the accuracies as the final accuracy score for the decision tree. Moving onto random forest which I found to be more effective then the decisions tree, I ended up using 15 estimators, which represented 15 different models. Next I implemented a random forest with bagging, which created additional data for training through using combinations with repetitions of data. This method improved random forest by 3%. But by far

the most effective classifier was the feedforward network with an overall accuracy of 84%. The model I ended up choosing was primarily using layers of dense and dropout layers. Dropout layers helping to prevent overfitting, and this was key to improving accuracy. For the last step I used a softmax activation function to instead of a relu because this model was not doing a binary classification but a classification of many cell types. Overall I found that the FFNN was the most effective model overall and is therefore the classifier I would use.