Final project

BIOENG 145, SP2021, Prof. Liana Lareau

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Setup

In [1]:

```
import numpy as np
import pandas as pd
import seaborn as sns
import tensorflow as tf
import tensorflow_probability as tfp
import matplotlib.pyplot as plt

# Part 1 dependencies
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE
from sklearn import random_projection
from sklearn.preprocessing import normalize
from sklearn.model_selection import train_test_split as split
tfd = tfp.distributions
tfpl = tfp.layers
keras = tf.keras
layers = tf.keras.layers

# Part 2 dependencies
from sklearn.ensemble import AdaBoostClassifier, RandomForestClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.multiclass import OneVsRestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.naive_bayes import MultinomialNB, ComplementNB
from sklearn.neural_network import MLPClassifier
from tabulate import tabulate
```

In [2]:

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

Part 0: Exploratory data analysis & preprocessing

0.1: Visualizing the tables

In [3]:

```
labels_pd.head()
```

Out[3]:

	index	bulk_labels
0	AAAGCCTGGCTAAC-1	CD14+ Monocyte
1	AAATTCGATGCACA-1	Dendritic
2	AACACGTGGTCTTT-1	CD56+ NK
3	AAGTGCACGTGCTA-1	CD4+/CD25 T Reg
4	ACACGAACGGAGTG-1	Dendritic

In [4]:

```
counts_pd.head()
```

Out[4]:

	Unnamed: 0	HES4	TNFRSF4	SSU72	PARK7	RBP7	SRM	MAD2L2	AGTRAP	TNFRSF1B	EFHD2	NECAP2	HP1BP
0	AAAGCCTGGCTAAC-1	-0.326	-0.191	-0.728	-0.301	3.386	-0.531	2.016	3.377	4.841	-0.525	-0.525	1.80
1	AAATTCGATGCACA-1	1.171	-0.191	0.795	-1.200	-0.174	-0.531	1.889	-0.486	-0.459	-0.525	1.287	-0.42
2	AACACGTGGTCTTT-1	-0.326	-0.191	0.483	-1.200	-0.174	-0.531	-0.451	0.971	-0.459	2.286	-0.525	1.25
3	AAGTGCACGTGCTA-1	-0.326	-0.191	1.134	-0.157	-0.174	-0.531	-0.451	-0.486	-0.459	-0.525	-0.525	9.90
4	ACACGAACGGAGTG-1	-0.326	-0.191	-0.728	-0.607	-0.174	-0.531	-0.451	0.787	-0.459	1.932	-0.525	1.04

5 rows × 766 columns

0.2: Visualize first 100 genes

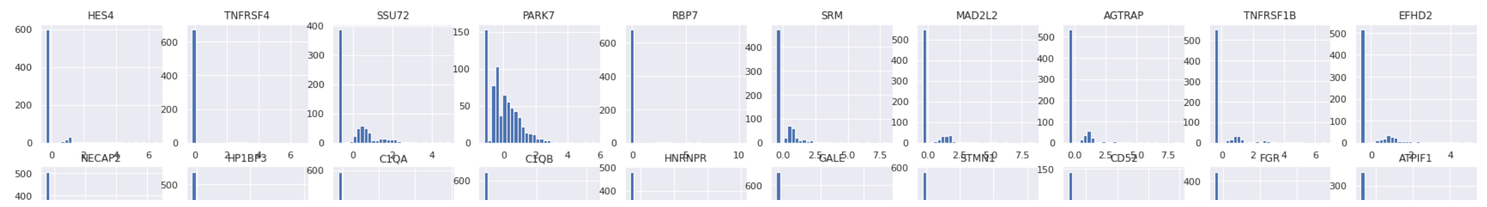
In [5]:

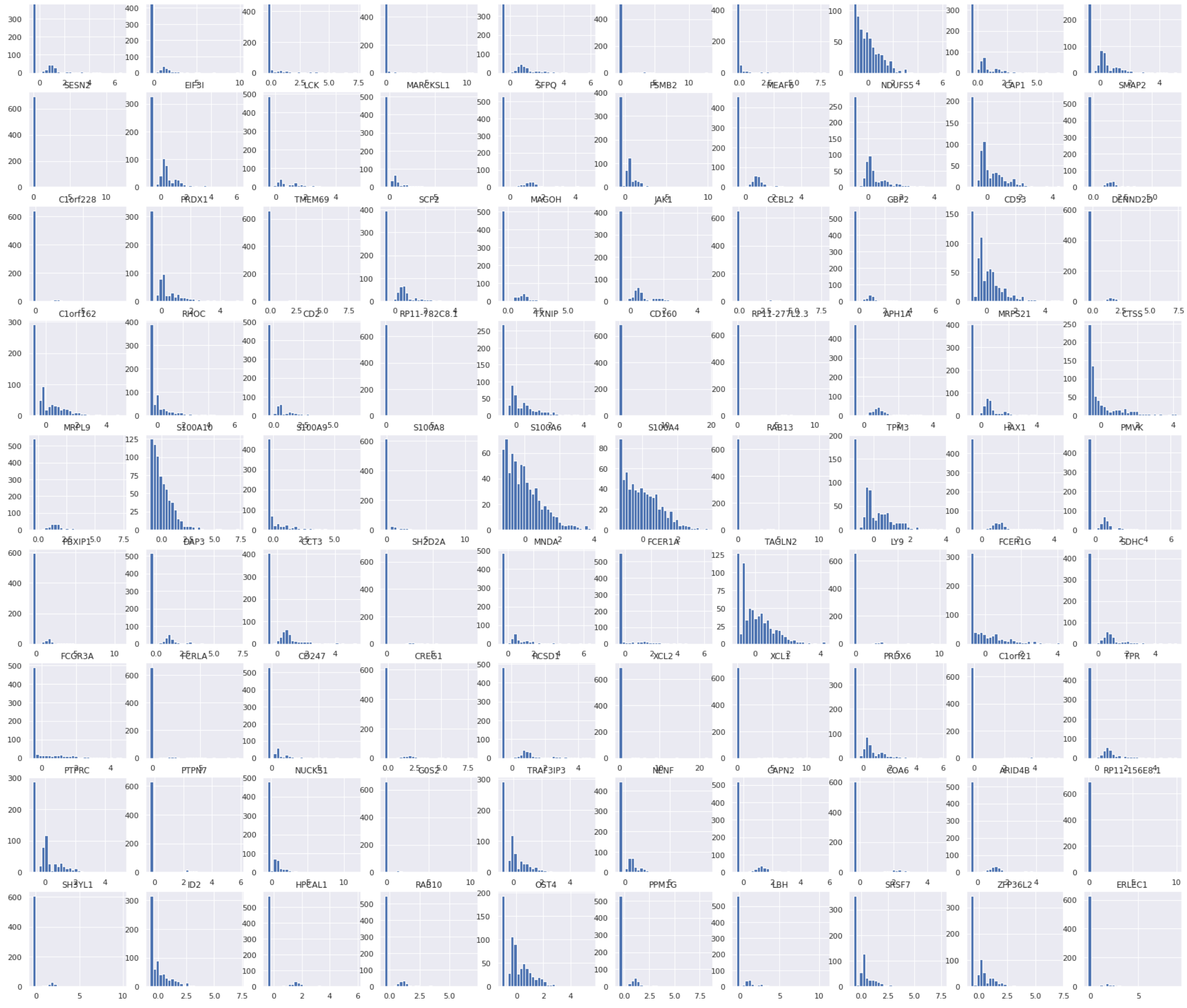
```
genes = list(counts_pd.columns)[1:]
barcodes = list(counts_pd["Unnamed: 0"])
unique_labels = labels_pd.bulk_labels.unique()
encode = {}
for i, l in enumerate(unique_labels):
    encode[l] = i

counts = counts_pd.to_numpy()
labels = labels_pd.to_numpy()[:, 1]
X = counts[:, 1:].astype(np.float64)
y = [encode[l] for l in labels]
num_samples, num_genes = X.shape
```

In [6]:

```
fig, ax = plt.subplots(10, 10, figsize=(30, 30))
for i in range(100):
    ax[i//10, i%10].hist(counts_pd.iloc[:,i+1], bins=30)
    ax[i//10, i%10].set_title(genes[i])
```





0.3: Visualize the correlation between gene counts

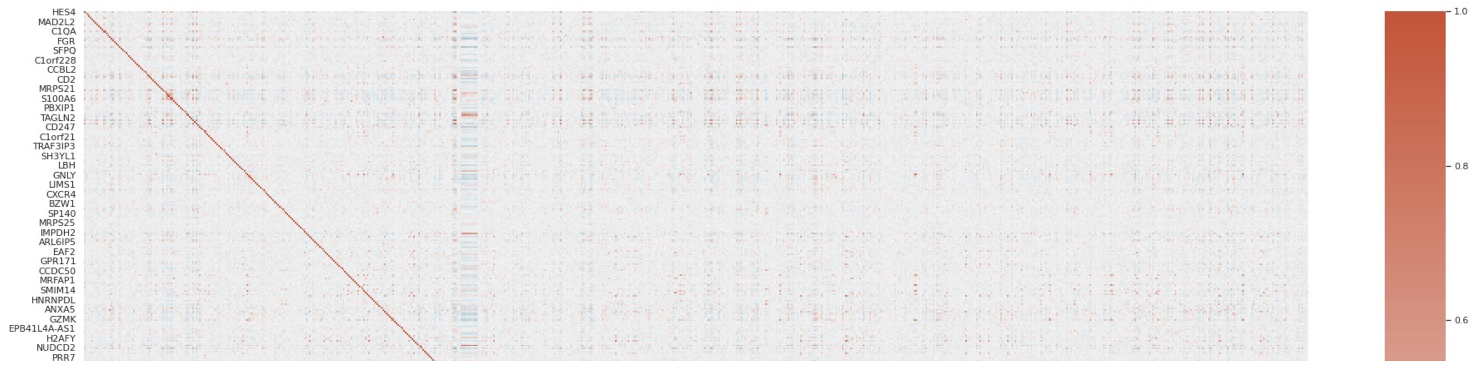
In [7]:

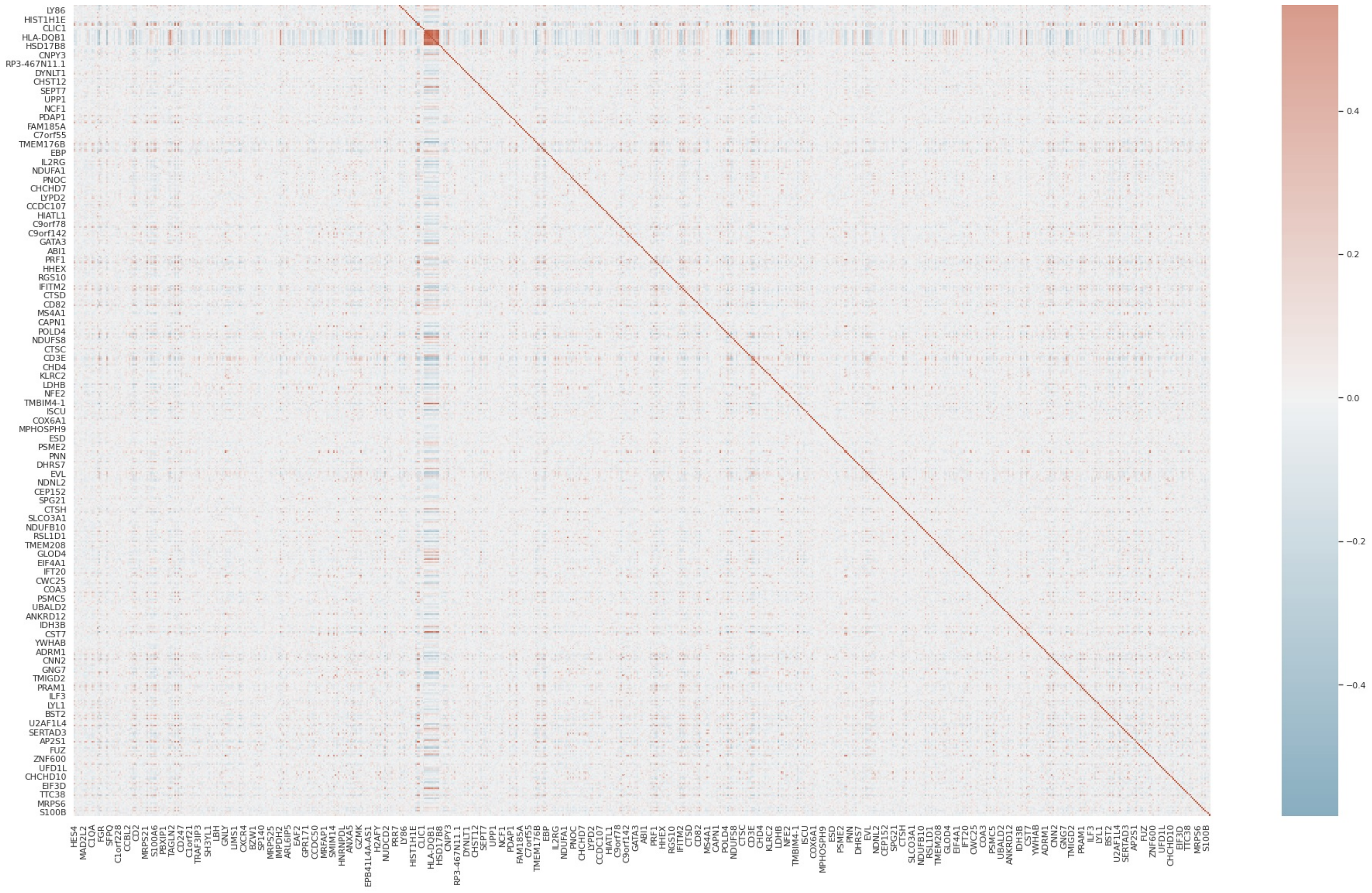
```
corr = counts_pd.corr()

f, ax = plt.subplots(figsize=(33, 27))
cmap = sns.diverging_palette(230, 20, as_cmap=True)
sns.heatmap(corr, cmap=cmap, center=0, square=True)
```

Out[7]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fe9e4eda050>
```





Part 1: Autoencoder

In [8]:

```python
# Check that we are using GPU for the runtime
if tf.test.gpu_device_name() != '/device:GPU:0':
    print('WARNING: GPU device not found.')
else:
    print('SUCCESS: Found GPU: {}'.format(tf.test.gpu_device_name()))
```

```
SUCCESS: Found GPU: /device:GPU:0
```

1.1: Building a variational autoencoder

In [9]:

```python
class Autoencoder(keras.Model):
    """
    Initializes a variational autoencoder with the following parameters:
    Parameters:
    - input_size: size of individial observations
    - latent_dim: size of the latent space
    - beta: reguarlization term for KL divergence
    """
    def __init__(self, input_size, latent_dim=32, beta=1):
        super(Autoencoder, self).__init__()
        self.latent_dim = latent_dim
        self.beta = beta

        self.encoder = self.build_encoder(input_size)
        self.mean = keras.Sequential([layers.Dense(latent_dim, name="mean")])
        self.log_var = keras.Sequential([layers.Dense(latent_dim, name="log_var", activatio
n='softplus')])
        self.decoder = self.build_decoder(input_size)

        self.loss_tracker = keras.metrics.Mean(name='loss')

    @property
    def metrics(self):
        return [
            self.loss_tracker
        ]

    """
    Helper function for adding dense layers to a NN.
    Parameters:
    - model: the Keras neural network
    - size: input size of the dense layer
    - drop: if not False, must be a number in (0, 1) specifying the dropout rate
    - l: multiplier for l1-regularization
    """
    def add_dense(self, m, size, activation='relu', drop=False, l=0.001):
        m.add(layers.Dense(size, activation=activation, activity_regularizer=keras.regulari
zers.L1(l1=l)))
        if drop:
            m.add(layers.Dropout(drop))

    """
    Builds the encoder portion of the autoencoder.
    Parameters:
    - input_size: dimensions of the initial input
    - latent_dim: size of the latent space, the output of the last layer
    """
    def build_encoder(self, input_size):
        e = keras.Sequential([layers.Input(shape=(input_size,))])
        e.add(layers.Flatten())
        e.add(keras.layers.GaussianNoise(1))
        self.add_dense(e, input_size)
        self.add_dense(e, 256, drop=0.4)
        self.add_dense(e, 128, drop=0.3)
        self.add_dense(e, 64, drop=0.2)
        return e

    """
    Bulds the decoder portion of the autoencoder.
    Parameters:
    - output_size: dimensions of the output
    - latent_dim: size of the latent space
    """
    def build_decoder(self, output_size):
        d = keras.Sequential([layers.Input(shape=(self.latent_dim,))])
        self.add_dense(d, self.latent_dim)
        self.add_dense(d, 64, drop=0.2)
        self.add_dense(d, 128, drop=0.3)
        self.add_dense(d, 256, drop=0.4)
        self.add_dense(d, output_size)
        return d

    """
    Samples from a multivariate normal distribution given by
    mean vector mu and covariance matrix with diagonal entries
    specified by log_sigma.
    """
    def sample(self, mu, log_sigma):
        batch = tf.shape(mu)[0]
        dim = tf.shape(mu)[1]
        epsilon = tf.keras.backend.random_normal(shape=(batch, dim))
        return mu + tf.exp(0.5 * log_sigma) * epsilon
    """
    Computes the reconstruction and KL divergence loss.
    """
    def full_loss(self, x_true, x_pred, mu, log_sigma):
        #cross_ent = keras.losses.binary_crossentropy(x_true, x_pred, from_logits=True)
        #cross_ent = tf.reduce_sum(cross_ent, axis=-1)
        kl = -0.5*tf.reduce_sum(1 + log_sigma - tf.square(mu) - tf.exp(log_sigma), axis=-1)
        return tf.reduce_mean(self.beta*kl + keras.metrics.MSE(x_true, x_pred))

    """
    Forward pass of the neural network.
    """
    @tf.function
    def call(self, x):
        e = self.encoder(x)
        mu = self.mean(e)
        log_sigma = self.log_var(e)
        z = self.sample(mu, log_sigma)
        return self.decoder(z), mu, log_sigma, z

    """
    Custom training function to implement the non-standard loss.
    """
    @tf.function
    def train_step(self, data):
        with tf.GradientTape() as tape:
            x_hat, mu, log_sigma, z = self.call(data)
            loss = self.full_loss(data, x_hat, mu, log_sigma)

        grads = tape.gradient(loss, self.trainable_weights)
        self.optimizer.apply_gradients(zip(grads, self.trainable_weights))
        self.loss_tracker.update_state(loss)
        return {"loss": self.loss_tracker.result()}
```

1.2: Training the model and hyperparameter search

In [10]:

```
# Train and validation split
X_train, X_val, y_train, y_val = split(X, y, test_size=0.2, random_state=145)
```

We are searching over the following hyperparameters for our model:

- **DIMS: dimensions of the latent space**
- **BETAS: regularization constants for KL divergence**

In [11]:

```
# Hyperparameters to optimize over
# DIMS: the dimension of the latent space
# BETAS: the regularization term for KL divergence
DIMS = [2, 8, 16, 32, 48, 64]
BETAS = [0.001, 0.01, 0.1, 0, 1, 10]
PARAMS = np.array(np.meshgrid(DIMS, BETAS)).T.reshape(-1, 2)
```

In [12]:

```
train_losses = []
val_losses = []
val_losses_mse = []

for i, param in enumerate(PARAMS):
    dim, beta = param
    dim = round(dim)
    print("Training an autoencoder with dim = {} and beta = {}".format(dim, beta))
    vae = Autoencoder(num_genes, latent_dim=dim, beta=beta)
    vae.compile(optimizer='adam')
    loss_train = vae.fit(X_train, batch_size=140, epochs=20, verbose=0)
    train_losses.append(loss_train.history['loss'][-1])

    x_hat, mu, log_sigma, z = vae.predict(X_val)
    loss_val = vae.full_loss(X_val, x_hat, mu, log_sigma)
    loss_val = loss_val.numpy()
    val_losses.append(loss_val)

    loss_mse = keras.losses.MSE(X_val, x_hat)
    loss_mse = np.mean(loss_mse.numpy())
    val_losses_mse.append(loss_mse)

    print("Validation loss (same metric as training): {}".format(loss_val))
    print("Validation loss (MSE): {}".format(loss_mse))
```

```
Training an autoencoder with dim = 2 and beta = 0.001
Validation loss (same metric as training): 1.023852825164795
Validation loss (MSE): 1.0211083889007568
Training an autoencoder with dim = 2 and beta = 0.01
Validation loss (same metric as training): 1.0317126512527466
Validation loss (MSE): 1.0316394567489624
Training an autoencoder with dim = 2 and beta = 0.1
Validation loss (same metric as training): 1.0325876474380493
Validation loss (MSE): 1.0316907167434692
Training an autoencoder with dim = 2 and beta = 0.0
Validation loss (same metric as training): 1.0041192770004272
Validation loss (MSE): 1.0041192770004272
Training an autoencoder with dim = 2 and beta = 1.0
Validation loss (same metric as training): 1.0389471054077148
Validation loss (MSE): 1.0315399169921875
Training an autoencoder with dim = 2 and beta = 10.0
Validation loss (same metric as training): 1.1013747453689575
Validation loss (MSE): 1.0315746068954468
Training an autoencoder with dim = 8 and beta = 0.001
Validation loss (same metric as training): 1.0054939985275269
Validation loss (MSE): 1.0008692741394043
Training an autoencoder with dim = 8 and beta = 0.01
Validation loss (same metric as training): 1.0322821140289307
Validation loss (MSE): 1.031759262084961
Training an autoencoder with dim = 8 and beta = 0.1
Validation loss (same metric as training): 1.0370362997055054
Validation loss (MSE): 1.0316104888916016
Training an autoencoder with dim = 8 and beta = 0.0
Validation loss (same metric as training): 0.9904032945632935
Validation loss (MSE): 0.9904032945632935
Training an autoencoder with dim = 8 and beta = 1.0
Validation loss (same metric as training): 1.0751137733459473
Validation loss (MSE): 1.0317806005477905
Training an autoencoder with dim = 8 and beta = 10.0
Validation loss (same metric as training): 1.4349397420883179
Validation loss (MSE): 1.0316162109375
Training an autoencoder with dim = 16 and beta = 0.001
Validation loss (same metric as training): 1.0161707401275635
Validation loss (MSE): 1.012373447418213
Training an autoencoder with dim = 16 and beta = 0.01
Validation loss (same metric as training): 1.0321656465530396
Validation loss (MSE): 1.0316157341003418
Training an autoencoder with dim = 16 and beta = 0.1
Validation loss (same metric as training): 1.0365846157073975
Validation loss (MSE): 1.031382441520691
Training an autoencoder with dim = 16 and beta = 0.0
Validation loss (same metric as training): 0.9801134467124939
Validation loss (MSE): 0.9801135659217834
Training an autoencoder with dim = 16 and beta = 1.0
Validation loss (same metric as training): 1.1300973892211914
Validation loss (MSE): 1.0316104888916016
Training an autoencoder with dim = 16 and beta = 10.0
Validation loss (same metric as training): 1.732474446296692
Validation loss (MSE): 1.0314873456954956
Training an autoencoder with dim = 32 and beta = 0.001
Validation loss (same metric as training): 1.0272231101989746
Validation loss (MSE): 1.025095820426941
Training an autoencoder with dim = 32 and beta = 0.01
Validation loss (same metric as training): 1.0322763919830322
Validation loss (MSE): 1.0314418077468872
Training an autoencoder with dim = 32 and beta = 0.1
Validation loss (same metric as training): 1.041706919670105
Validation loss (MSE): 1.0314915180206299
Training an autoencoder with dim = 32 and beta = 0.0
Validation loss (same metric as training): 0.9800335764884949
Validation loss (MSE): 0.9800334572792053
Training an autoencoder with dim = 32 and beta = 1.0
Validation loss (same metric as training): 1.122320532798767
Validation loss (MSE): 1.0315625667572021
Training an autoencoder with dim = 32 and beta = 10.0
Validation loss (same metric as training): 1.9930980205535889
Validation loss (MSE): 1.0315146446228027
Training an autoencoder with dim = 48 and beta = 0.001
Validation loss (same metric as training): 1.0317589044570923
Validation loss (MSE): 1.0315203666687012
Training an autoencoder with dim = 48 and beta = 0.01
Validation loss (same metric as training): 1.0330359935760498
Validation loss (MSE): 1.0315765142440796
Training an autoencoder with dim = 48 and beta = 0.1
Validation loss (same metric as training): 1.0456730127334595
Validation loss (MSE): 1.0314431190490723
Training an autoencoder with dim = 48 and beta = 0.0
Validation loss (same metric as training): 0.9722540974617004
Validation loss (MSE): 0.9722540974617004
Training an autoencoder with dim = 48 and beta = 1.0
Validation loss (same metric as training): 1.1549530029296875
Validation loss (MSE): 1.0314594507217407
Training an autoencoder with dim = 48 and beta = 10.0
Validation loss (same metric as training): 2.2848784923553467
Validation loss (MSE): 1.031363606452942
Training an autoencoder with dim = 64 and beta = 0.001
Validation loss (same metric as training): 1.031600832939148
Validation loss (MSE): 1.0314089059829712
Training an autoencoder with dim = 64 and beta = 0.01
Validation loss (same metric as training): 1.033061146736145
Validation loss (MSE): 1.0314265489578247
Training an autoencoder with dim = 64 and beta = 0.1
Validation loss (same metric as training): 1.0438786745071411
Validation loss (MSE): 1.0314562320709229
Training an autoencoder with dim = 64 and beta = 0.0
Validation loss (same metric as training): 0.974838376045227
Validation loss (MSE): 0.9748384952545166
Training an autoencoder with dim = 64 and beta = 1.0
Validation loss (same metric as training): 1.2265604734420776
Validation loss (MSE): 1.0314619541168213
Training an autoencoder with dim = 64 and beta = 10.0
Validation loss (same metric as training): 2.7642765045166016
Validation loss (MSE): 1.0313963890075684
```

In [13]:

```
# Determine best parameters
val_losses_mse = np.array(val_losses_mse)
best_idx = np.argmin(val_losses_mse)
dim = round(PARAMS[best_idx][0])
beta = PARAMS[best_idx][1]
print("Best parameters: dim = {}, beta = {}".format(dim, beta))
```

```
Best parameters: dim = 48, beta = 0.0
```

1.3: Evaluating the model

1.3.1: PCA

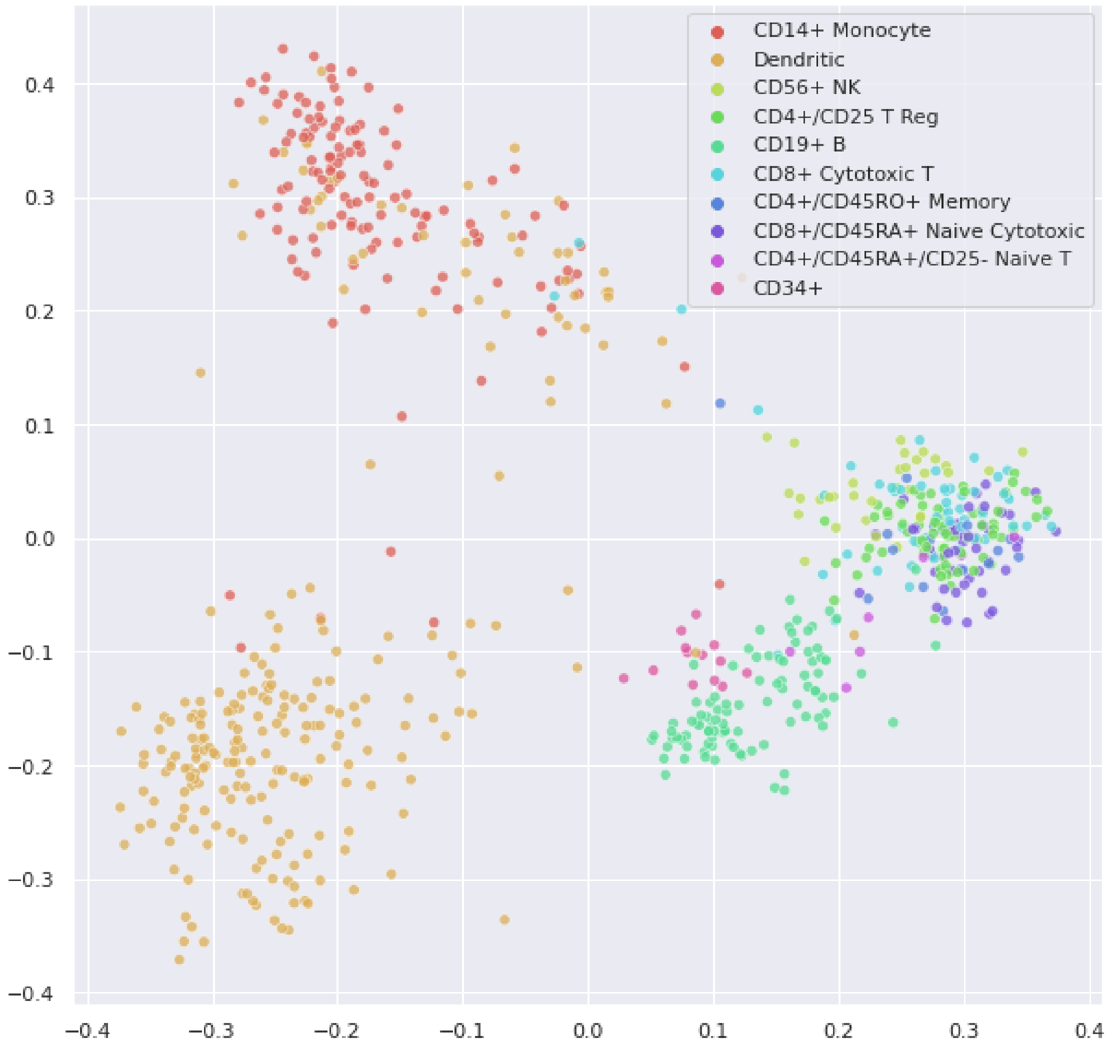
In [14]:

```
X_norm = normalize(X)
X_pca = PCA(n_components=2).fit_transform(X_norm)

plt.figure(figsize=(10, 10))
ax = sns.scatterplot(
    x=X_pca[:,0], y=X_pca[:,1],
    hue=y,
    palette=sns.color_palette("hls", len(unique_labels)),
    legend='full',
    alpha=0.75
)
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles, unique_labels, loc='upper right')
```

Out[14]:

```
<matplotlib.legend.Legend at 0x7fe974284790>
```



1.3.2: tSNE

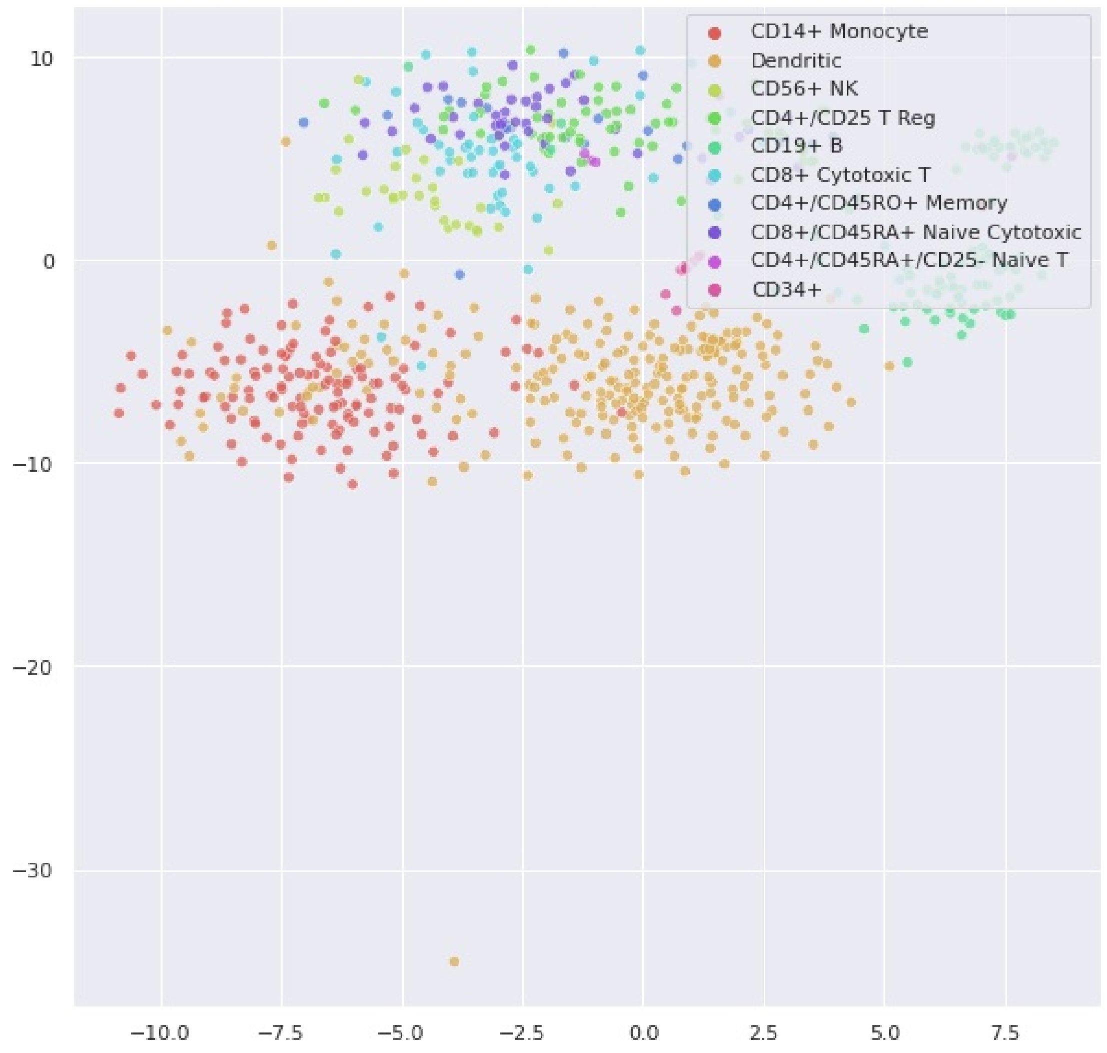
In [15]:

```
X_tsne = TSNE(n_components=2, perplexity=30).fit_transform(X)

plt.figure(figsize=(10, 10))
ax = sns.scatterplot(
    x=X_tsne[:,0], y=X_tsne[:,1],
    hue=y,
    palette=sns.color_palette("hls", len(unique_labels)),
    legend='full',
    alpha=0.75
)
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles, unique_labels, loc='upper right')
```

Out[15]:

```
<matplotlib.legend.Legend at 0x7fe9743744d0>
```



1.3.3: Random projections

1.3.3.1: Sparse random projection

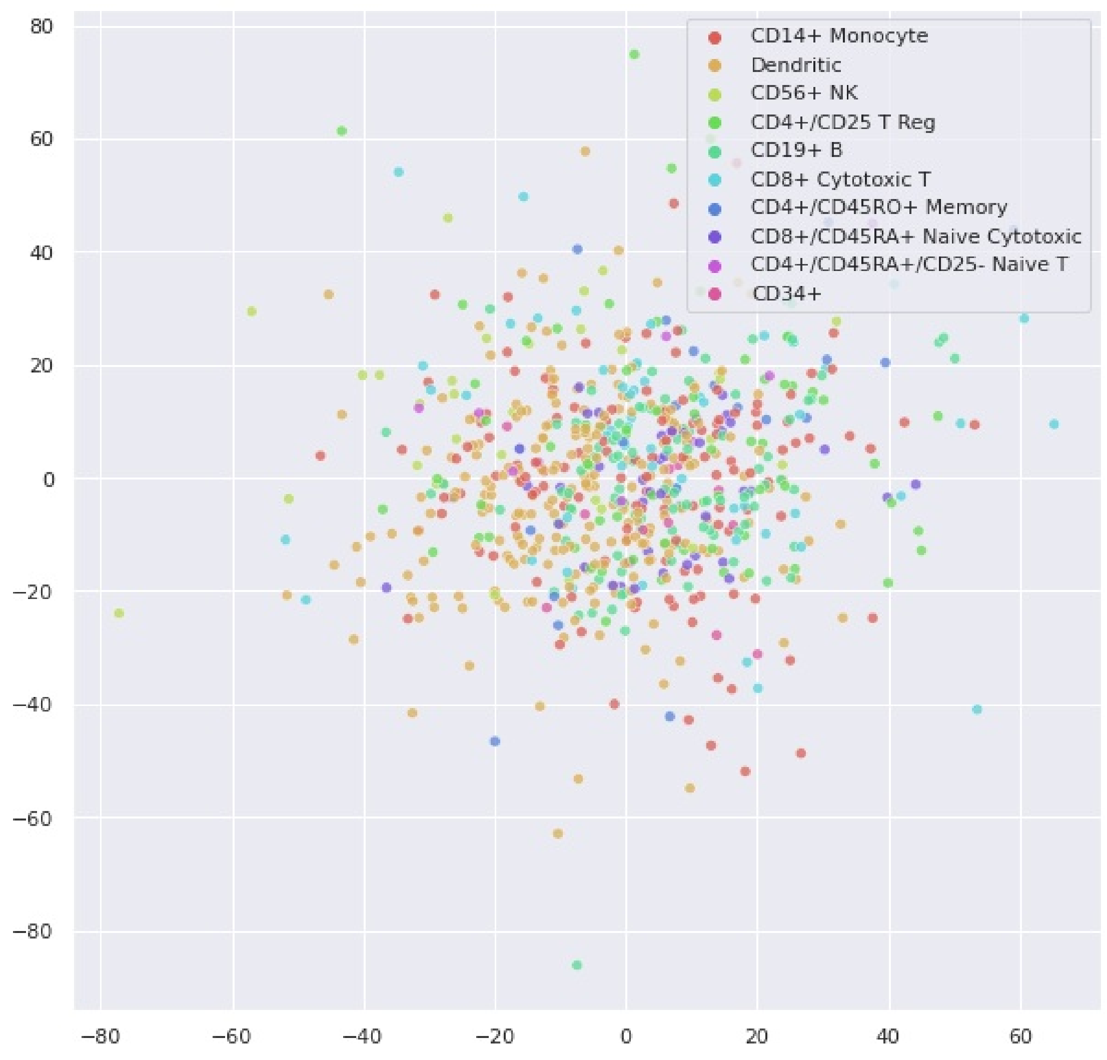
In [16]:

```
X_sparse = random_projection.SparseRandomProjection(n_components=2).fit_transform(X)

plt.figure(figsize=(10, 10))
ax = sns.scatterplot(
    x=X_sparse[:,0], y=X_sparse[:,1],
    hue=y,
    palette=sns.color_palette("hls", len(unique_labels)),
    legend='full',
    alpha=0.75
)
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles, unique_labels, loc='upper right')
```

Out[16]:

```
<matplotlib.legend.Legend at 0x7fe974779c50>
```



1.3.3.2: Gaussian random projection

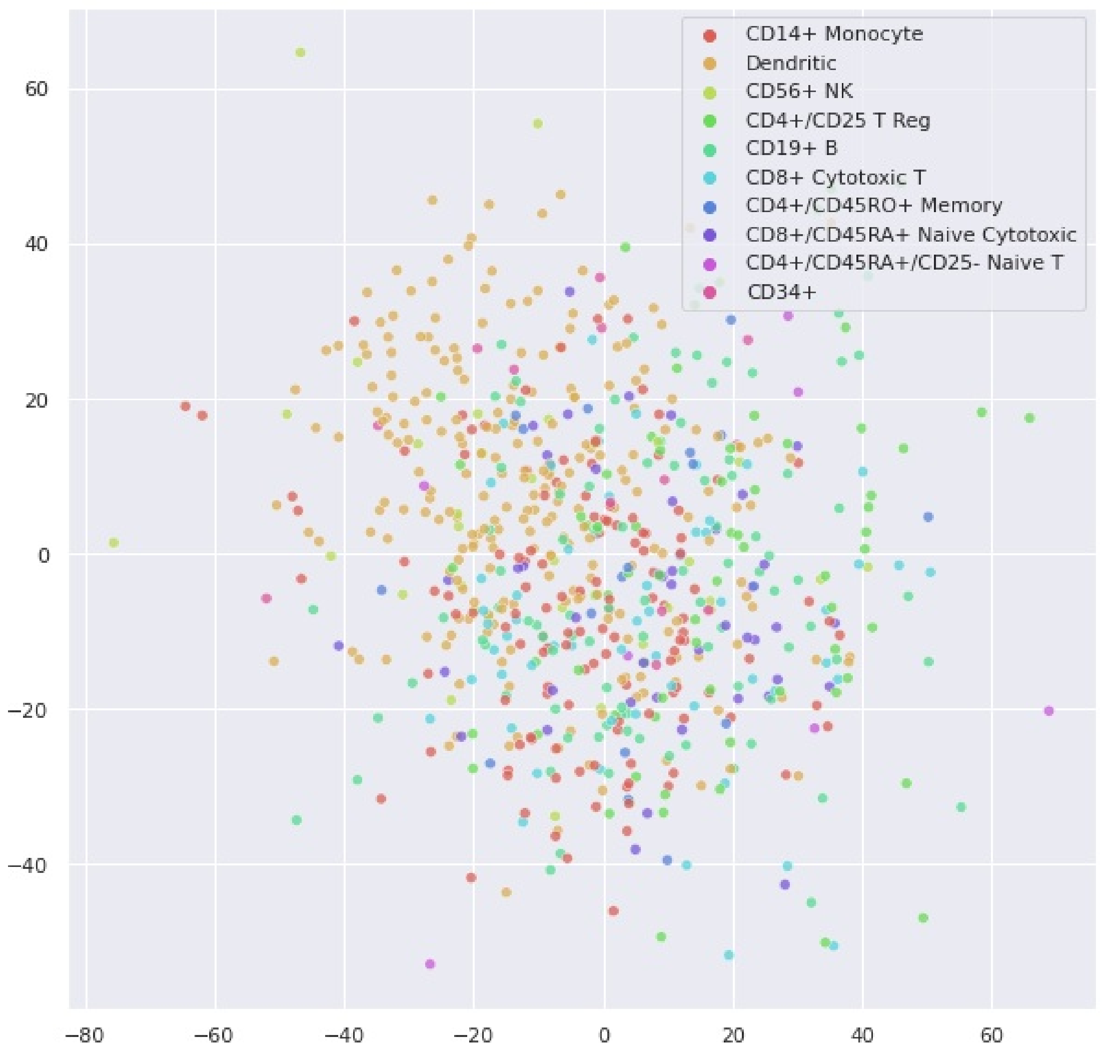
In [17]:

```
X_gauss = random_projection.GaussianRandomProjection(n_components=2).fit_transform(X)

plt.figure(figsize=(10, 10))
ax = sns.scatterplot(
    x=X_gauss[:,0], y=X_gauss[:,1],
    hue=y,
    palette=sns.color_palette("hls", len(unique_labels)),
    legend='full',
    alpha=0.75
)
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles, unique_labels, loc='upper right')
```

Out[17]:

```
<matplotlib.legend.Legend at 0x7fe962628710>
```



1.3.4: Autoencoder

1.3.4.1: Autoencoder on best parameters

In [18]:

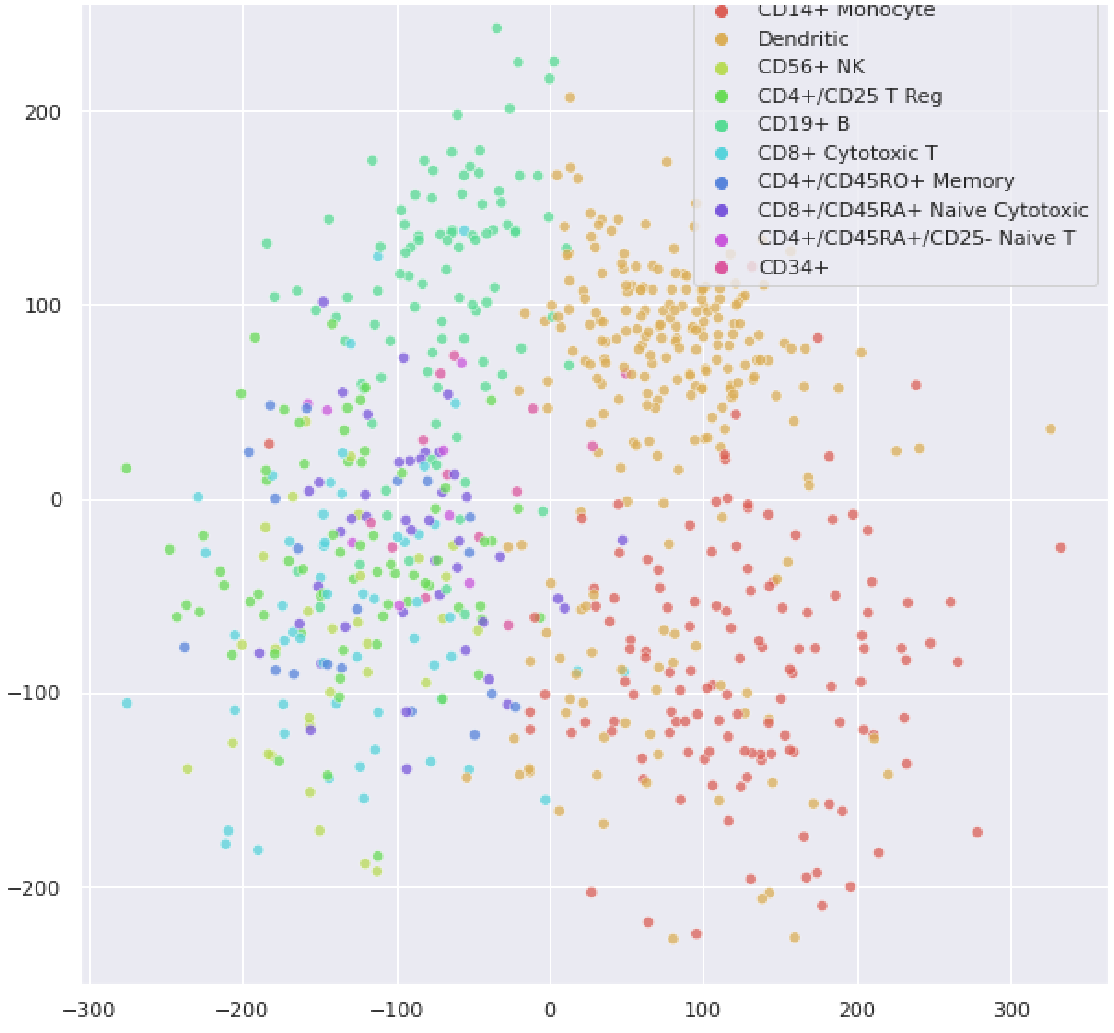
```
# Autoencoder latent space + PCA on best determined parameters
vae_best = Autoencoder(num_genes, latent_dim=dim, beta=beta)
vae_best.compile(optimizer='adam')
vae_best.fit(X, batch_size=70, epochs=100, verbose=0);
```

In [19]:

```
_, _, _, X_vae_best = vae_best.predict(X)

X_vae_best_pca = PCA(n_components=2).fit_transform(X_vae_best)

plt.figure(figsize=(10, 10))
ax = sns.scatterplot(
    x=X_vae_best_pca[:,0], y=X_vae_best_pca[:,1],
    hue=y,
    palette=sns.color_palette("hls", len(unique_labels)),
    legend='full',
    alpha=0.75
)
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles, unique_labels, loc='upper right');
```



1.3.4.2: Autoencoder on different parameters

In [20]:

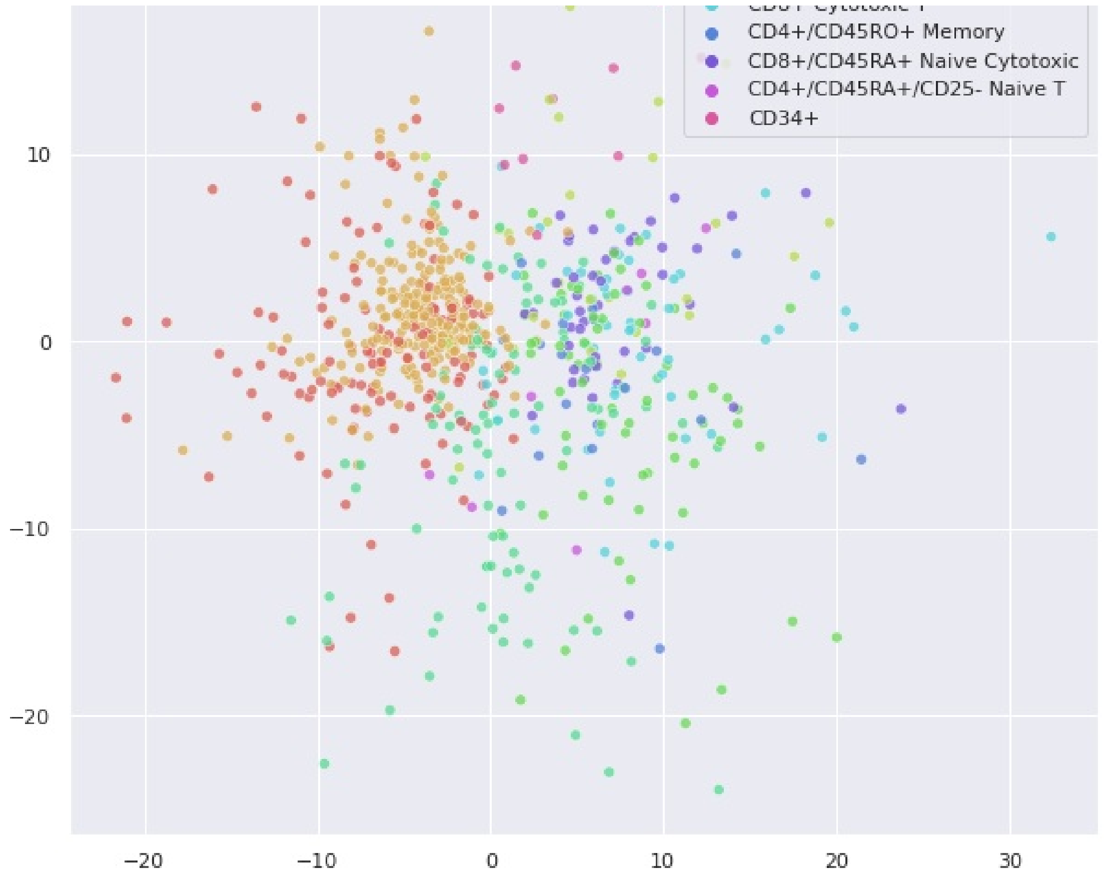
```
# Autoencoder latent space + PCA on different parameters
vae_alt = Autoencoder(num_genes, latent_dim=8, beta=0.0001)
vae_alt.compile(optimizer='adam')
vae_alt.fit(X, batch_size=70, epochs=100, verbose=0);
```

In [21]:

```
_, _, _, X_vae_alt = vae_alt.predict(X)

X_vae_alt_pca = PCA(n_components=2).fit_transform(X_vae_alt)

plt.figure(figsize=(10, 10))
ax = sns.scatterplot(
    x=X_vae_alt_pca[:,0], y=X_vae_alt_pca[:,1],
    hue=y,
    palette=sns.color_palette("hls", len(unique_labels)),
    legend='full',
    alpha=0.75
)
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles, unique_labels, loc='upper right');
```



1.3.4.3: Autoencoder on 2-dimensions

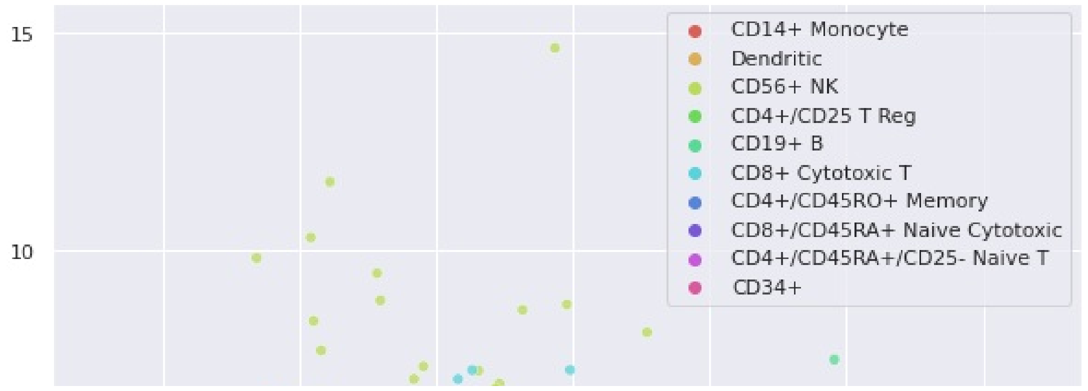
In [22]:

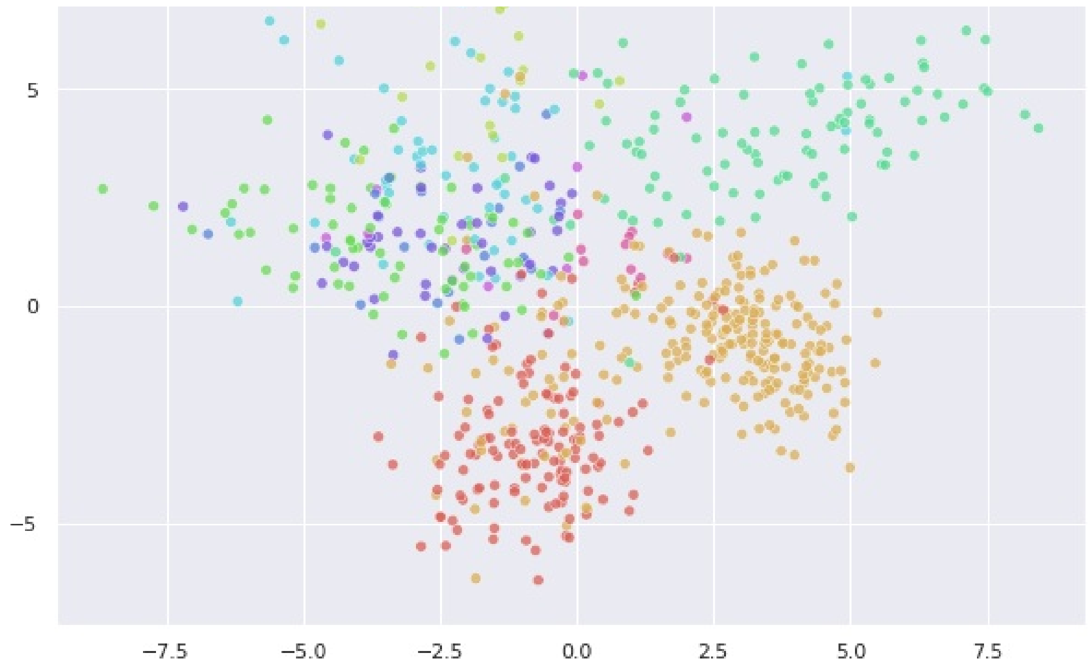
```
# Autoencoder with 2-dimensional latent space
vae_small = Autoencoder(num_genes, latent_dim=2, beta=0.001)
vae_small.compile(optimizer='adam')
vae_small.fit(X, batch_size=70, epochs=100, verbose=0);
```

In [23]:

```
_, _, _, X_vae_small = vae_small.predict(X)

plt.figure(figsize=(10, 10))
ax = sns.scatterplot(
    x=X_vae_small[:,0], y=X_vae_small[:,1],
    hue=y,
    palette=sns.color_palette("hls", len(unique_labels)),
    legend='full',
    alpha=0.75
)
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles, unique_labels, loc='upper right');
```





1.3.4.4: Writeup

While PCA and tSNE seem to lead to better separation (clearer clusters) in the data qualitatvely, we see that the autoencoder performs favorably compared to the two and seems to outperform random projection methods. For downstream analysis such as k-means clustering or classification, PCA and tSNE appear to be the superior methods. However, there is still value in the autoencoder. Since the variational autoencoder is a generative model, unlike PCA and tSNE, it can be used for tasks such as synthetic datasets, imputation, etc. Much like tSNE, we can also adjust the parameters in our model to get different types of clusters in our projection (namely, by changing the value of β).

Part 2: Classifier

In this section of the project, we try out the following classifiers and report on their validation accuracy:

- **Single decision tree**
- **Random forest**
- **AdaBoost on shallow decision trees**
- **Support vector machines**
- **Multinomial naive Bayes**
- **Complement naive Bayes**
- **Logistic regression**
- **Out-of-the-box MLP**
- **Custom MLP**

2.1: Decision trees

2.1.1: Single large decision tree

In [24]:

```
single_tree = DecisionTreeClassifier(criterion='entropy');
single_tree.fit(X_train, y_train);
```

In [25]:

```
single_tree_score = single_tree.score(X_val, y_val)
single_tree_table = ['Decision tree', single_tree_score]
print("Validation accuracy of a single decision tree: {}".format(single_tree_score))
```

```
Validation accuracy of a single decision tree: 0.6785714285714286
```

A single decision tree provides a good baseline for validation accuracy. We see that for this model, the accuracy is quite poor.

2.1.2: Random forest

In [26]:

```
random_forest = RandomForestClassifier(n_estimators=1000, criterion='entropy', max_depth=8)
random_forest.fit(X_train, y_train);
```

In [27]:

```
random_forest_score = random_forest.score(X_val, y_val)
random_forest_table = ['Random forest', random_forest_score]
print("Validation accuracy of a random forest: {}".format(random_forest_score))
```

```
Validation accuracy of a random forest: 0.7928571428571428
```

When we introduce some bagging and randomization, we can improve the accuracy by quite a bit, almost reaching our threshold of 0.80.

2.1.3: AdaBoost with shallow decision trees

In [28]:

```
base_tree = DecisionTreeClassifier(criterion='entropy', max_depth=4)
boosted_forest = AdaBoostClassifier(base_estimator=base_tree, n_estimators=1000, random_stat
e=145);
boosted_forest.fit(X_train, y_train);
```

In [29]:

```
boosted_forest_score = boosted_forest.score(X_val, y_val)
boosted_forest_table = ['AdaBoost w/ shallow decision trees', boosted_forest_score]
print("Validation accuracy of a boosted forest: {}".format(boosted_forest_score))
```

```
Validation accuracy of a boosted forest: 0.8
```

Taking this further with boosting, we see that once again we are very close to our threshold. However, it might be the case that the model is overfitting, or that decision trees are not well suited for our data.

2.2: Support vector machines

In [30]:

```
base_svm = SVC(C=0.01, kernel='linear')
svms = OneVsRestClassifier(base_svm);
svms.fit(X_train, y_train);
```

In [31]:

```
svms_score = svms.score(X_val, y_val)
svms_table = ['SVMs', svms_score]
print("Validation accuracy of multiple SVMSs: {}".format(svms_score))
```

```
Validation accuracy of multiple SVMSs: 0.8714285714285714
Validation accuracy of multiple SVMss: 0.8714285714285714
```

SVMs seem to work suprisingly well on our data, suggesting that linear boundaries are well-suited in this context.

2.3: Naive Bayes

We can also attempt to model the data in a more probabilistic manner, which yields decent results.

In [32]:

```
X_train_shifted = X_train - np.min(X_train, axis=0)
mt_bayes = MultinomialNB(alpha=10)
mt_bayes.fit(X_train_shifted, y_train);
```

In [33]:

```
X_val_shifted = X_val - np.min(X_val, axis=0)
mt_bayes_score = mt_bayes.score(X_val_shifted, y_val)
mt_bayes_table = ['Multinomial Bayes', mt_bayes_score]
print("Validation accuracy of multinomial naive Bayes: {}".format(mt_bayes_score))
```

```
Validation accuracy of multinomial naive Bayes: 0.8285714285714286
```

In [34]:

```
comp_bayes = ComplementNB(alpha=1)
comp_bayes.fit(X_train_shifted, y_train);
```

In [35]:

```
comp_bayes_score = comp_bayes.score(X_val_shifted, y_val)
comp_bayes_table = ['Complement Bayes', comp_bayes_score]
print("Validation accuracy of complement naive Bayes: {}".format(comp_bayes_score))
```

```
Validation accuracy of complement naive Bayes: 0.8
```

2.4: Logistic regression

In [36]:

```
base_logistic = LogisticRegression(C=100, multi_class='multinomial')
logistics = OneVsRestClassifier(base_logistic)
logistics.fit(X_train, y_train);
```

In [37]:

```
logistics_score = logistics.score(X_val, y_val)
logistics_table = ['Logistic regression', logistics_score]
print("Validation accuracy of logistic regression: {}".format(logistics_score))
```

```
Validation accuracy of logistic regression: 0.8642857142857143
```

We see that logistic regression has good validation accuracy, once again suggesting that the decision boundaries roughly linear.

2.5: Neural network

In [38]:

```
# Check that we are using GPU for the runtime
if tf.test.gpu_device_name() != '/device:GPU:0':
    print('WARNING: GPU device not found.')
else:
    print('SUCCESS: Found GPU: {}'.format(tf.test.gpu_device_name()))
```

```
SUCCESS: Found GPU: /device:GPU:0
```

2.5.1: Out-of-the-box MLP

In [39]:

```
mlp = MLPClassifier()
mlp.fit(X_train, y_train);
```

In [40]:

```
ootb_mlp_score = mlp.score(X_val, y_val)
ootb_mlp_table = ['Out-of-the-box MLP', ootb_mlp_score]
print("Validation accuracy of an out-of-the-box MLP: {}".format(ootb_mlp_score))
```

```
Validation accuracy of an out-of-the-box MLP: 0.8142857142857143
```

An out-of-the-box seems to work well, but not as well as other, simpler methods such as SVMs or logistic regression. This might be due to overfitting due to the parameters in neural networks. Maybe we can achieve better accuracy with a custom MLP.

2.5.2: Custom MLP

In [68]:

```
# One-hot encoding
num_cats = len(unique_labels)
y_hot = np.zeros((num_samples, num_cats))
for i in range(num_samples):
    y_hot[i, y[i]] = 1
```

In [69]:

```
# Train/test split
X_train, X_test, y_train, y_test = split(X, y_hot, test_size=0.2, random_state=145)
```

In [100]:

```
clf = keras.Sequential([layers.Input(shape=(num_genes,))])

clf.add(layers.GaussianNoise(1))

clf.add(layers.Dense(512, activation='relu', activity_regularizer=keras.regularizers.L2(l2=
0.001)))
clf.add(layers.Dropout(rate=0.4))

clf.add(layers.Dense(128, activation='relu', activity_regularizer=keras.regularizers.L2(l2=
0.001)))
clf.add(layers.Dropout(rate=0.3))

clf.add(layers.Dense(32, activation='relu'))

clf.add(layers.Dense(num_cats, activation='softmax'))
```

In [101]:

```
optimizer = keras.optimizers.Adam(learning_rate=0.001)
clf.compile(optimizer=optimizer, loss='categorical_crossentropy', metrics='categorical_accur
acy')
```

In [104]:

```
num_epochs = 50
clf.fit(X_train, y_train, batch_size=70, epochs=num_epochs, verbose=0);
```

In [105]:

```
custom_mlp_score = clf.evaluate(X_test, y_test)[1]
custom_mlp_table = ['Custom MLP', custom_mlp_score]
print("Validation accuracy of custom MLP: {}".format(custom_mlp_score))
```

```
5/5 [==============================] - 0s 3ms/step - loss: 0.8395 - categorical_accuracy: 0.
8286
Validation accuracy of custom MLP: 0.8285714387893677
```

2.6: Summary of classifiers + writeup

In [106]:

```
data = [
        single_tree_table,
        random_forest_table,
        boosted_forest_table,
        svms_table,
        mt_bayes_table,
        comp_bayes_table,
        logistics_table,
        ootb_mlp_table,
        custom_mlp_table
]
header = ["Model", "Validation accuracy"]
print(tabulate(data, headers=header))
```

```
Model                                  Validation accuracy
-----------------------------------  ---------------------
Decision tree                                     0.678571
Random forest                                     0.792857
AdaBoost w/ shallow decision trees                0.8
SVMs                                              0.871429
Multinomial Bayes                                 0.828571
Complement Bayes                                  0.8
Logistic regression                               0.864286
Out-of-the-box MLP                                0.814286
Custom MLP                                        0.828571
```

Therefore, the classifier of choice is the support vector machine with linear kernel. One possible reason as to why this classifier works well is because the data is inherently linearly separable. Recalling the visualizations in 0.2, we notice that many of the gene counts congregate towards 0, while a couple have higher values. In other words, the data is naturally sparse. This means that we can draw a threshold value for each gene count to divide those cells with no expression of the gene and those with high expression. Because of this, a clasifier with linear decision boundaries is a good fit. This idea is further supported by the high validation accuracy of logistic regression, which can also find linear decision boundaries. On the other hand, methods such as decision trees and naive Bayes do not necessarily find a linear hypothesis.