In [6]:
```
import pandas as pd
import numpy as np
from sklearn.preprocessing import StandardScaler
from sklearn.manifold import TSNE
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import cross_validate, StratifiedKFold, train_
from sklearn.svm import SVC
from sklearn.naive_bayes import GaussianNB
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import confusion_matrix
import seaborn as sns
%matplotlib inline
import matplotlib.pyplot as plt
# from tpot import TPOTClassifier
# from xgboost import XGBClassifier
```

Load Data

In [7]:
```
nt_all = pd.read_csv('data/nt.all.csv')
```

In [8]:
```
nt_coding = pd.read_csv('data/nt.coding.csv')
```

In [9]:
```
nt_all.head()
```

Out[9]:

	Type	ENSG00000000003.13	ENSG00000000005.5	ENSG00000000419.11	ENSG00000000457.12	ENS
0	0	150265.480539	4327.845865	713909.310619	59794.653619	
1	0	913228.181789	2326.284691	828500.414250	50302.756694	
2	0	359658.934678	228971.470681	483960.593070	69872.468893	
3	1	135634.675596	0.000000	748257.784782	75504.611322	
4	0	81454.831124	177.310309	363281.940134	45622.048124	

5 rows × 60484 columns

In [10]:
```
nt_all.shape
```

Out[10]: (1400, 60484)

In [11]:
```
nt_coding.head()
```

Out[11]:

	Type	ENSG00000000003.13	ENSG00000000005.5	ENSG00000000419.11	ENSG00000000457.12	ENS
0	0	150265.480539	4327.845865	713909.310619	59794.653619	
1	0	913228.181789	2326.284691	828500.414250	50302.756694	
2	0	359658.934678	228971.470681	483960.593070	69872.468893	
3	1	135634.675596	0.000000	748257.784782	75504.611322	
4	0	81454.831124	177.310309	363281.940134	45622.048124	

5 rows × 19562 columns

In [12]:
```
nt_coding.shape
```

Out[12]:
```
(1400, 19562)
```

Pre-processing

Seperate labels and features

In [13]:
```
y_coding = nt_coding['Type']
X_coding = nt_coding.drop('Type', axis=1)
```

In [14]:
```
y_all = nt_all['Type']
X_all = nt_all.drop('Type', axis=1)
```

Split into training and validation sets

In [15]:
```
X_coding_train, X_coding_test, y_coding_train, y_coding_test = train_test_s
                                                        test_size=.25, random_s
```

In [16]:
```
X_all_train, X_all_test, y_all_train, y_all_test = train_test_split(X_all,
                                                        test_size=.25, random_s
```

In [34]:
```
scaler_coding = StandardScaler()
scaler_all = StandardScaler()

X_coding_train = scaler_coding.fit_transform(X_coding_train)
X_coding_test = scaler_coding.transform(X_coding_test)

X_all_train = scaler_all.fit_transform(X_all_train)
X_all_test = scaler_all.transform(X_all_test)
```

Classification

- k-nearest neighbors
- Support Vector Machine (SVM)
- Naive Bayes
- Decision Tree
- Random Forest

In [35]:
```
def display_cv_metrics(metrics):
    for k, v in metrics.items():
        print(f'{k}: {np.round(v.mean(), 3)}')
```

In [36]:
```
metrics = ['accuracy', 'f1', 'precision', 'recall', 'roc_auc']
```

In [38]:
```
skf = StratifiedKFold(n_splits=5, random_state=1, shuffle=True)
```

k-nearest neighbors

In [40]:
```
knn = KNeighborsClassifier()
```

In [41]:
```
knn_scores_coding = cross_validate(estimator=knn,
                                   X=X_coding_train,
                                   y=y_coding_train,
                                   scoring=metrics,
                                   cv=skf)
```

In [42]:
```
knn_scores_all = cross_validate(estimator=knn,
                                X=X_all_train,
                                y=y_all_train,
                                scoring=metrics,
                                cv=skf)
```

In [43]:
```
display_cv_metrics(knn_scores_coding)
```

```
fit_time: 0.81
score_time: 11.025
test_accuracy: 0.891
test_f1: 0.882
test_precision: 0.982
test_recall: 0.802
test_roc_auc: 0.966
```

In [44]:
```
display_cv_metrics(knn_scores_all)
```

```
fit_time: 3.364
score_time: 32.006
test_accuracy: 0.841
test_f1: 0.817
test_precision: 0.984
test_recall: 0.7
test_roc_auc: 0.956
```

Support Vector Machine

In [97]:
```
svc = SVC(kernel='linear')
```

In [98]:
```
svc_scores_coding = cross_validate(estimator=svc,
                                   X=X_coding_train,
                                   y=y_coding_train,
                                   scoring=metrics,
                                   cv=skf)
```

In [99]:
```
svc_scores_all = cross_validate(estimator=svc,
                                X=X_all_train,
                                y=y_all_train,
                                scoring=metrics,
                                cv=skf)
```

In [100]:
```
display_cv_metrics(svc_scores_coding)
```

```
fit_time: 4.691
score_time: 2.066
test_accuracy: 0.972
test_f1: 0.973
test_precision: 0.98
test_recall: 0.966
test_roc_auc: 0.992
```

In [101]:
```
display_cv_metrics(svc_scores_all)
```

```
fit_time: 20.542
score_time: 9.303
test_accuracy: 0.972
test_f1: 0.973
test_precision: 0.981
test_recall: 0.965
test_roc_auc: 0.993
```

Naive Bayes Classifier

In [50]:
```
nb = GaussianNB()
```

In [51]:
```
nb_scores_coding = cross_validate(estimator=nb,
                                  X=X_coding_train,
                                  y=y_coding_train,
                                  scoring=metrics,
                                  cv=skf)
```

In [73]:
```
nb_scores_all = cross_validate(estimator=nb,
                               X=X_all_train,
                               y=y_all_train,
                               scoring=metrics,
                               cv=skf)
```

In [53]:
```
display_cv_metrics(nb_scores_coding)
```

```
fit_time: 0.444
score_time: 0.095
test_accuracy: 0.918
test_f1: 0.921
test_precision: 0.91
test_recall: 0.933
test_roc_auc: 0.922
```

In [74]:
```
display_cv_metrics(nb_scores_all)
```

```
fit_time: 2.445
score_time: 0.309
test_accuracy: 0.657
test_f1: 0.708
test_precision: 0.629
test_recall: 0.812
test_roc_auc: 0.654
```

Decision Tree Classifier

In [55]:
```
dt = DecisionTreeClassifier(random_state=1)
```

In [56]:
```
dt_scores_coding = cross_validate(estimator=dt,
                                  X=X_coding_train,
                                  y=y_coding_train,
                                  scoring=metrics,
                                  cv=skf)
```

In [57]:
```
dt_scores_all = cross_validate(estimator=dt,
                               X=X_all_train,
                               y=y_all_train,
                               scoring=metrics,
                               cv=skf)
```

In [58]:
```
display_cv_metrics(dt_scores_coding)
```

```
fit_time: 6.907
score_time: 0.02
test_accuracy: 0.909
test_f1: 0.91
test_precision: 0.914
test_recall: 0.907
test_roc_auc: 0.909
```

In [59]:
```
display_cv_metrics(dt_scores_all)
```

```
fit_time: 14.78
score_time: 0.06
test_accuracy: 0.905
test_f1: 0.906
test_precision: 0.913
test_recall: 0.899
test_roc_auc: 0.905
```

Random Forest Classifier

In [60]:
```
rf = RandomForestClassifier(max_depth=3, random_state=1)
```

In [61]:
```
rf_scores_coding = cross_validate(estimator=rf,
                                  X=X_coding_train,
                                  y=y_coding_train,
                                  scoring=metrics,
                                  cv=skf)
```

In [62]:
```
rf_scores_all = cross_validate(estimator=rf,
                               X=X_all_train,
                               y=y_all_train,
                               scoring=metrics,
                               cv=skf)
```

In [63]:
```
display_cv_metrics(rf_scores_coding)
```

```
fit_time: 1.971
score_time: 0.037
test_accuracy: 0.957
test_f1: 0.958
test_precision: 0.956
test_recall: 0.961
test_roc_auc: 0.991
```

In [64]:
```
display_cv_metrics(rf_scores_all)
```

```
fit_time: 3.422
score_time: 0.067
test_accuracy: 0.956
test_f1: 0.957
test_precision: 0.961
test_recall: 0.953
test_roc_auc: 0.992
```

Selecting the best performer

In [65]:
```
scores_all = [knn_scores_all, svc_scores_all, nb_scores_all,
              dt_scores_all, rf_scores_all]

scores_coding = [knn_scores_coding, svc_scores_coding,
                 nb_scores_coding, dt_scores_coding, rf_scores_coding]

names = ['K-Nearest Neighbors', 'Support Vector Classifier', 'Naive Bayes C
         'Decision Tree Classifier', 'Random Forest Classifier']
```

In [66]:
```
for score in scores_all:
    for k, v in score.items():
        score[k] = v.mean()
```

In [67]:
```
for score in scores_coding:
    for k, v in score.items():
        score[k] = v.mean()
```

For all genes

In [109]:
```
pd.DataFrame(scores_all, index=names)
```

Out[109]:

	fit_time	score_time	test_accuracy	test_f1	test_precision	test_recall	test_roc_auc
K-Nearest Neighbors	3.364365	32.006083	0.840952	0.816745	0.984169	0.699533	0.955647
Support Vector Classifier	20.541505	9.303161	0.972381	0.972630	0.981336	0.964521	0.992669
Naive Bayes Classifier	2.191593	0.295318	0.657143	0.707806	0.629284	0.811578	0.653981
Decision Tree Classifier	14.779774	0.060417	0.904762	0.905943	0.912786	0.899290	0.904899
Random Forest Classifier	3.422036	0.067356	0.956190	0.956934	0.960781	0.953340	0.992069

For only protein-coding genes

In [110]:
```
pd.DataFrame(scores_coding, index=names)
```

Out[110]:

	fit_time	score_time	test_accuracy	test_f1	test_precision	test_recall	test_roc_auc
K-Nearest Neighbors	0.809870	11.025419	0.891429	0.882157	0.981738	0.802077	0.965718
Support Vector Classifier	4.690663	2.065730	0.972381	0.972663	0.979575	0.966390	0.992378
Naive Bayes Classifier	0.443795	0.095060	0.918095	0.920576	0.909718	0.932866	0.921958
Decision Tree Classifier	6.906948	0.019686	0.908571	0.910091	0.913765	0.906819	0.908616
Random Forest Classifier	1.971109	0.036887	0.957143	0.958180	0.956230	0.960782	0.991180

Important RNA-sequences in Classifying Tumor

Support Vector Classifier with linear kernel seems to have a slightly higher cross validated ROC AUC and accuracy scores across both datasets, closely followed by the Random Forest Classifier.

Dataset with just the protein-coding genes seems to be performing as well as the full dataset despite having fewer features. We will compute Random Forest feature importances based on mean decrease in impurity and display the first 10 genes that are the best predictors of tumor.

Random Forest Feature Importances

In [76]:
```
rf.fit(X_all_train, y_all_train)
```

Out[76]:
```
RandomForestClassifier(max_depth=3, random_state=1)
```

In [77]:
```
importances = rf.feature_importances_
```

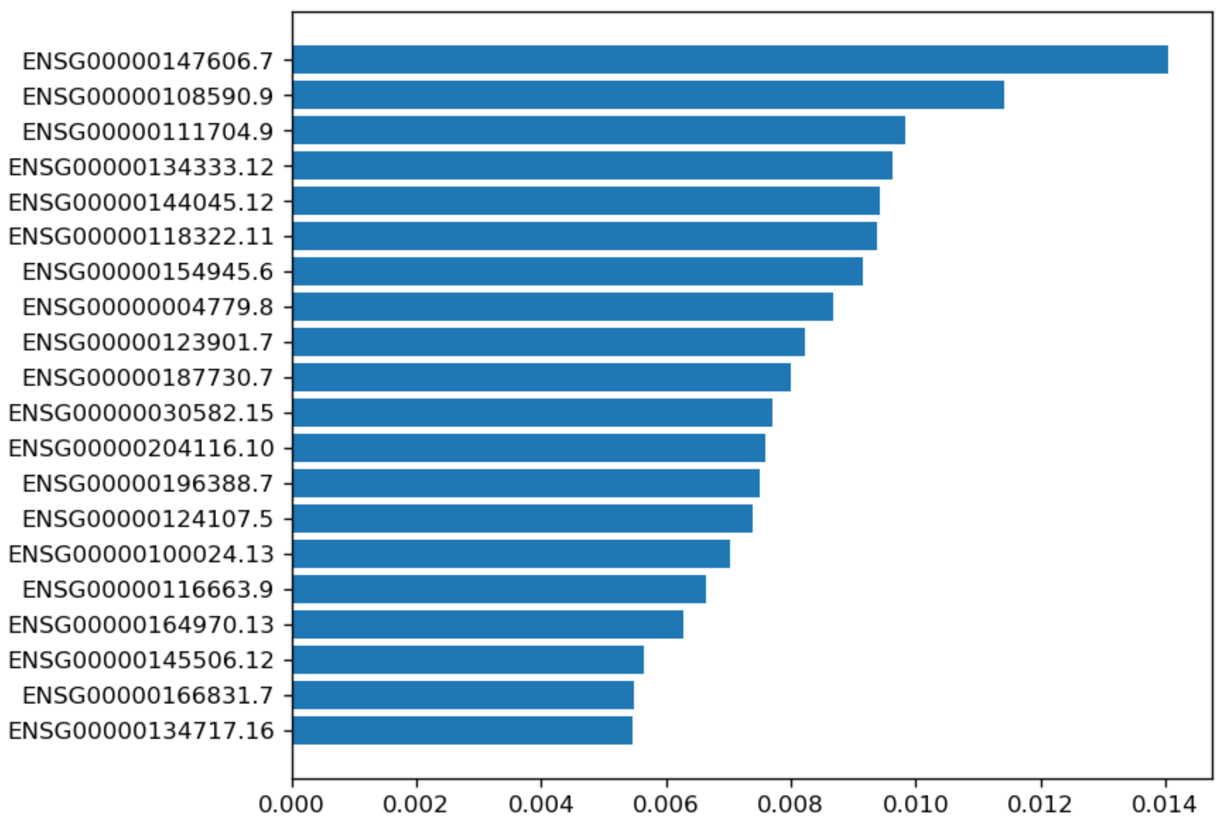
In [78]:
```
feature_names = list(nt_coding.columns[1:])
```

In [79]:
```
importance_df = pd.DataFrame(zip(feature_names, importances), columns=['gen
```

Top 20 genes for predicting tumor

In [191]:
```
top_20_rf = importance_df.sort_values('importance', ascending=False).head(2
```

In [194]:
```
plt.figure(figsize=(7, 6), dpi=120)
plt.barh(y=top_20_rf.gene[::-1], width=top_20_rf.importance[::-1]);
```



SVC Feature Importances

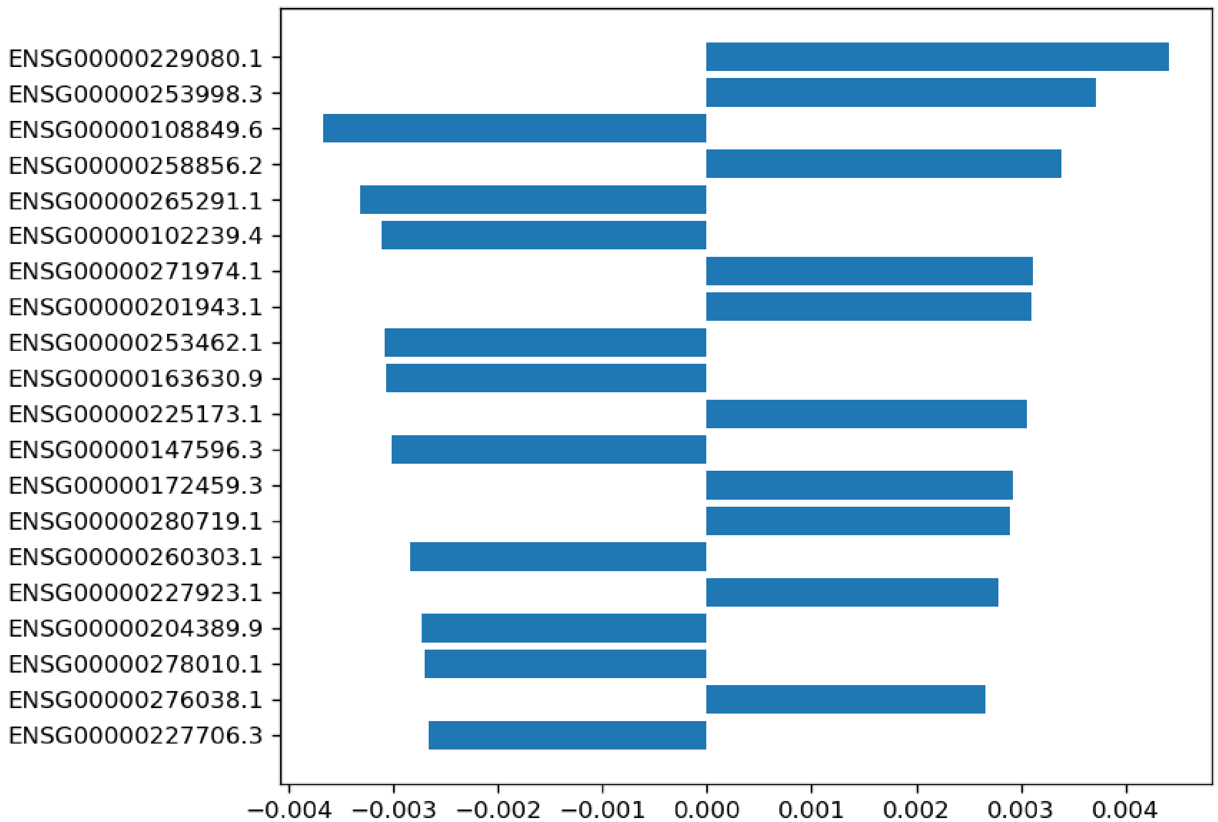
In [111]:
```
svc = SVC(kernel='linear')
svc.fit(X_all_train, y_all_train)
```

Out[111]:
```
SVC(kernel='linear')
```

In [175]:
```
names, imp = zip(*sorted(zip(nt_all.columns[1:], svc.coef_[0]), key=lambda
```

Highest coefficients where higher absolute value means more influence on the decision of the classifier:

In [198]:
```
plt.figure(figsize=(7, 6), dpi=120)
plt.barh(y=names[-20:], width=imp[-20:]);
```



Check to see if any common features for SVC and Random Forest in the top 20:

In [206]:
```
set(names[-20:]) & set(top_20_rf.gene)
```

Out[206]:
```
set()
```

Nope.

Confusion matrix with the predictions on the holdout set

Random Forest

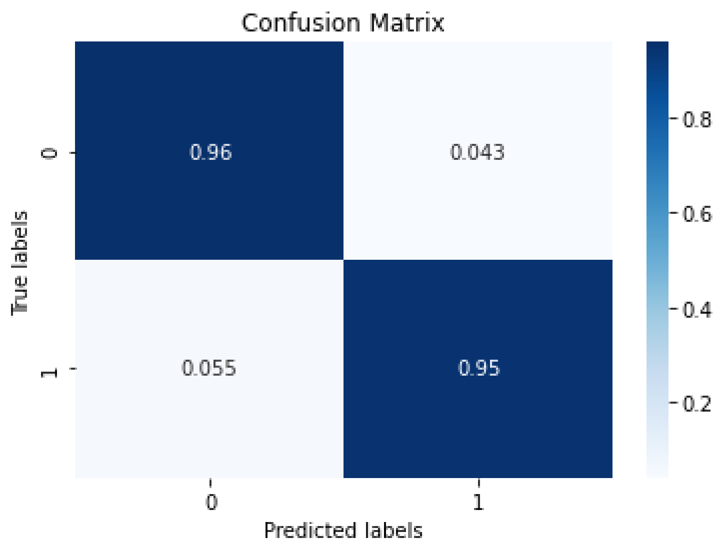
In [210]:
```
y_all_pred = rf.predict(X_all_test)
```

In [211]:
```
cf_matrix = confusion_matrix(y_all_test, y_all_pred, normalize='true')
```

In [213]:
```
test_accuracy = (y_all_pred == y_all_test).sum() / len(y_all_test)
print(f"Test accuracy is {test_accuracy * 100}%")
```

```
Test accuracy is 95.14285714285714%
```

In [214]:
```
ax = plt.axes()
sns.heatmap(cf_matrix, annot=True, cmap='Blues', ax=ax)
ax.set_title('Confusion Matrix')
ax.set_xlabel('Predicted labels')
ax.set_ylabel('True labels');
```



Support Vector Machine

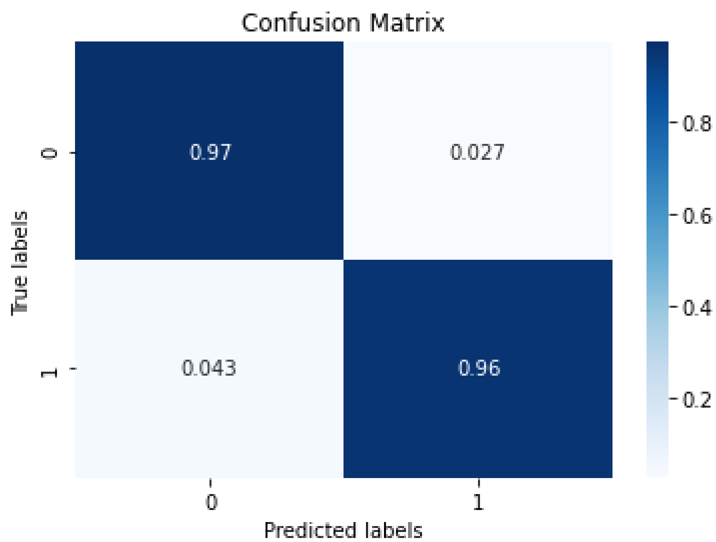
In [215]:
```
y_all_pred = svc.predict(X_all_test)
```

In [216]:
```
cf_matrix = confusion_matrix(y_all_test, y_all_pred, normalize='true')
```

In [217]:
```
test_accuracy = (y_all_pred == y_all_test).sum() / len(y_all_test)
print(f"Test accuracy is {test_accuracy * 100}%")
```

```
Test accuracy is 96.57142857142857%
```

In [218]:
```
ax = plt.axes()
sns.heatmap(cf_matrix, annot=True, cmap='Blues', ax=ax)
ax.set_title('Confusion Matrix')
ax.set_xlabel('Predicted labels')
ax.set_ylabel('True labels');
```



Deep Learning Classifier

In [1]:
```
import keras
from keras.layers import Input, Dense
from keras.models import Model
```

In [21]:
```
input_layer = Input(shape=(19561,))
dense = Dense(8192, activation='relu')(input_layer)
dense = Dense(2048, activation='relu')(input_layer)
dense = Dense(512, activation='relu')(input_layer)
dense = Dense(128, activation='relu')(input_layer)
dense = Dense(64, activation='relu')(dense)
dense = Dense(32, activation='relu')(dense)
dense = Dense(8, activation='relu')(dense)
output = Dense(1, activation='sigmoid')(dense)
```

In [22]:
```
model = Model(input_layer, output)
```

In [23]:
```
model.compile(loss='binary_crossentropy', optimizer='adam', metrics=['accur
```

In [30]:
```
test_sizes = np.arange(0.05, 0.8, 0.05)
learning_dict = {'Test sizes': test_sizes,
                 'Accuracy': [],
                 'Loss': [],
                 'AUC': []}

random_weights = model.get_weights()
for size in test_sizes:
    model.set_weights(random_weights)
    X_coding_train, X_coding_test, y_coding_train, y_coding_test = train_te
                                                        test_size=.25, rand
    scaler = StandardScaler()
    X_coding_train = scaler.fit_transform(X_coding_train)
    X_coding_test = scaler.transform(X_coding_test)

    model.fit(X_coding_train, y_coding_train, epochs=100,
       batch_size=20)
    loss, accuracy, auc = model.evaluate(X_coding_test, y_coding_test, verb
    learning_dict['Loss'].append(loss)
    learning_dict['Accuracy'].append(accuracy)
    learning_dict['AUC'].append(auc)
```

```
Epoch 1/100
53/53 [==============================] - 0s 6ms/step - loss: 0.5584 - a
ccuracy: 0.6610 - auc: 0.7505
Epoch 2/100
53/53 [==============================] - 0s 5ms/step - loss: 0.5395 - a
ccuracy: 0.6838 - auc: 0.7626
Epoch 3/100
53/53 [==============================] - 0s 5ms/step - loss: 0.5190 - a
ccuracy: 0.6848 - auc: 0.7749
Epoch 4/100
53/53 [==============================] - 0s 5ms/step - loss: 0.5076 - a
ccuracy: 0.6981 - auc: 0.7988
Epoch 5/100
53/53 [==============================] - 0s 5ms/step - loss: 0.4973 - a
ccuracy: 0.7038 - auc: 0.8091
Epoch 6/100
53/53 [==============================] - 0s 5ms/step - loss: 0.4868 - a
ccuracy: 0.7076 - auc: 0.8193
Epoch 7/100
```

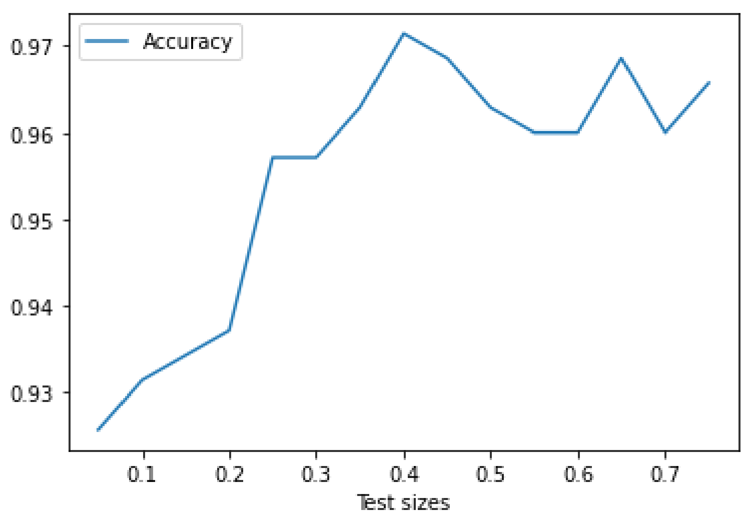
Learning Curve

In [37]:
```
learning_df
```

Out[37]:

	Test sizes	Accuracy	Loss	AUC
0	0.05	0.925714	0.510010	0.956825
1	0.10	0.931429	0.710257	0.953400
2	0.15	0.934286	0.364858	0.970873
3	0.20	0.937143	0.490639	0.967381
4	0.25	0.957143	0.474641	0.966726
5	0.30	0.957143	0.609394	0.967889
6	0.35	0.962857	0.968809	0.965087
7	0.40	0.971429	0.969524	0.976118
8	0.45	0.968571	0.566424	0.975741
9	0.50	0.962857	0.687308	0.967545
10	0.55	0.960000	0.541426	0.975446
11	0.60	0.960000	0.771379	0.970397
12	0.65	0.968571	0.656924	0.975856
13	0.70	0.960000	0.720427	0.967939
14	0.75	0.965714	0.348426	0.978708

In [35]:
```
learning_df = pd.DataFrame(learning_dict)
learning_df[['Test sizes', 'Accuracy']].plot(x='Test sizes');
```



Test accuracy peaks at 97.14 when we use 40% of the data for testing and 60% for training. Which is higher than the best performing traditinoal ML methods Support Vector Machine and Random Forest.

In [38]:
```
model.set_weights(random_weights)
X_coding_train, X_coding_test, y_coding_train, y_coding_test = train_test_s
                                                                test_size=.4, rando
scaler = StandardScaler()
X_coding_train = scaler.fit_transform(X_coding_train)
X_coding_test = scaler.transform(X_coding_test)

model.fit(X_coding_train, y_coding_train, epochs=100,
       batch_size=20)
```

```
Epoch 1/100
42/42 [==============================] - 0s 5ms/step - loss: 0.4058 - a
ccuracy: 0.7786 - auc: 0.8987
Epoch 2/100
42/42 [==============================] - 0s 5ms/step - loss: 0.1972 - a
ccuracy: 0.9167 - auc: 0.9812
Epoch 3/100
42/42 [==============================] - 0s 5ms/step - loss: 0.1784 - a
ccuracy: 0.9393 - auc: 0.9805
Epoch 4/100
42/42 [==============================] - 0s 5ms/step - loss: 0.1447 - a
ccuracy: 0.9417 - auc: 0.9846
Epoch 5/100
42/42 [==============================] - 0s 5ms/step - loss: 0.1005 - a
ccuracy: 0.9512 - auc: 0.9917
Epoch 6/100
42/42 [==============================] - 0s 5ms/step - loss: 0.0877 - a
ccuracy: 0.9536 - auc: 0.9928
Epoch 7/100
```

In [45]:
```
y_coding_pred == y_coding_test
```

...

Confusion Matrix for the Deep Learning Classifier

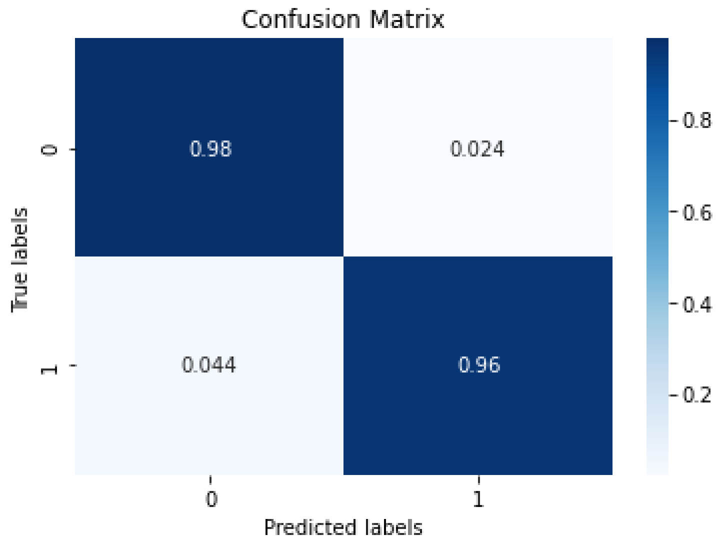
In [76]:
```
y_coding_pred = (model.predict(X_coding_test) > .5).reshape(560)

cf_matrix = confusion_matrix(y_coding_test, y_coding_pred, normalize='true'

test_accuracy = (y_coding_pred == y_coding_test).sum() / len(y_coding_test)
print(f"Test accuracy is {test_accuracy * 100}%")

ax = plt.axes()
sns.heatmap(cf_matrix, annot=True, cmap='Blues', ax=ax)
ax.set_title('Confusion Matrix')
ax.set_xlabel('Predicted labels')
ax.set_ylabel('True labels');
```

```
Test accuracy is 96.60714285714286%
```



Slightly different accuracy score.