W207.6 Final Project - Predicting Cancer Type from Tumor Mutations

Notebook 4 - Visualize Performance

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Initialization

In [0]:
```
import pandas as pd
import urllib.request
import numpy as np
import glob
import os
import warnings
from textwrap import wrap
import matplotlib.pyplot as plt
from IPython.display import display
import time
from IPython.core.interactiveshell import InteractiveShell

from sklearn import preprocessing
from sklearn import metrics
from sklearn.metrics import precision_recall_fscore_support
from sklearn.metrics import accuracy_score
from sklearn.metrics import confusion_matrix


InteractiveShell.ast_node_interactivity = "all"
plt.rcParams.update({'figure.max_open_warning': 0})

# Establish the colors for each cancer type
label_colors = []
cm = plt.get_cmap('tab20b')
for i in range(20):
    label_colors.append(cm(i))
cm = plt.get_cmap('tab20c')
for i in range(13):
    label_colors.append(cm(i))
```

In [0]:
```
# create the directory where the downloaded directory is stored
data_dir = "./data"
if not os.path.isdir(data_dir):
    os.makedirs(data_dir)

# create the directory where the metrics are stored
metrics_dir = "./metrics"
if not os.path.isdir(metrics_dir):
    os.makedirs(metrics_dir)

# create the raw where the source data is stored
raw_dir = "./raw"
if not os.path.isdir(raw_dir):
    os.makedirs(raw_dir)
```

In [0]:
```
# This downloads a dictionary file
dictionary_filename = "./raw/tcga_dictionaries.txt"
if os.path.isfile(dictionary_filename):
    print("Skipping download, as file %s is present" %(dictionary_filename))
else:
    print('Downloading dictionary file...')
    url = 'https://w207-final-project.s3.amazonaws.com/raw/tcga_dictionaries.txt'
    urllib.request.urlretrieve(url, dictionary_filename)
print("done.")


# This loads the data dictionary to will convert
# the tumor_sample_barcode into a cancer_type
# and provide full names for the cancer types
tcga_dict = open("./raw/tcga_dictionaries.txt","r")
dict_name_index = 0 #Set dictionary index counter to 0
for line in tcga_dict:
    if line.startswith("#"): #If line starts with #, the next line will be a known dictionary
        dict_name_index += 1
    elif dict_name_index == 4:
        tissue_source_site = eval(line)
    elif dict_name_index == 5:
        code_to_disease = eval(line)
    elif dict_name_index == 6:
        disease_to_code = eval(line)
```

```
Skipping download, as file ./raw/tcga_dictionaries.txt is present
done.
```

Visualize Performance across different feature sets, different classifiers

In [0]:
```
def get_saved_metrics():
    metrics_filename = "./metrics/metrics.csv"
    if os.path.isfile(metrics_filename):
        metrics_df = pd.read_csv(metrics_filename)
        metrics =  [row for row in metrics_df.T.to_dict().values()]
        return metrics
    else:
        return []

def get_saved_metrics_dataframe():
    metrics_filename = "./metrics/metrics.csv"
    if os.path.isfile(metrics_filename):
        metrics_df = pd.read_csv(metrics_filename)
        return metrics_df
    else:
        return None

def save_metrics(name, classifier, metrics, prf_by_label, confusion_mx):

    metrics_df = pd.DataFrame(metrics, columns=['name', 'classifier', 'feature_size',
                                                'accuracy', 'precision', 'recall', 'f1',
                                                'time'])

    # Write out scores as csv files
    metrics_df.to_csv("./metrics/metrics.csv")

    # Write out confusion matrix to csv file
    confusion_mx_df = pd.DataFrame.from_dict(confusion_mx)
    filename = "./metrics/confusion_" + name + "_" + classifier + ".csv"
    confusion_mx_df.to_csv(filename)

    # Write out precision, recall, f1 by class to csv file
    prf_by_label_df = pd.DataFrame(prf_by_label)
    prf_by_label_list = []
    for row in prf_by_label:
      prf_by_label_list.append(list(row))
    prf_by_label_df = pd.DataFrame(prf_by_label_list)
    filename = "./metrics/prf_by_class_" + name + "_" + classifier + ".csv"
    prf_by_label_df.to_csv(filename)

def get_prf_by_label(name, classifier):
    filename = "./metrics/prf_by_class_" + name + "_" + classifier + ".csv"
    if os.path.isfile(filename):
        prf_by_label_df = pd.read_csv(filename)
        return prf_by_label_df[prf_by_label_df.columns[1:]]
    else:
        return None

def get_confusion_matrix(name, classifier):
    filename = "./metrics/confusion_" + name + "_" + classifier + ".csv"
    if os.path.isfile(filename):
        confusion_df = pd.read_csv(filename)
        return confusion_df[confusion_df.columns[1:]]
    else:
        return None

def calculate_metrics(name, classifier, feature_size, predict, test_labels,
                      elapsed_time, metrics):
    # Get precision, recall, f1 scores
    prf_scores          = precision_recall_fscore_support(test_labels, predict,
                                                          average='weighted')
    acc_score           = accuracy_score(test_labels, predict)
    prf_by_label        = precision_recall_fscore_support(test_labels, predict,
                                                          average=None)
    classification_rpt  = classification_report(test_labels, predict)

    # Get confusion matrix
    conf_mx             = confusion_matrix(test_labels, predict)

    metrics.append({
     'name':               name,
     'classifier':         classifier,
     'feature_size':       feature_size,
     'accuracy':           acc_score,
     'precision':          prf_scores[0],
     'recall':             prf_scores[1],
     'f1':                 prf_scores[2],
     'time':               elapsed_time
    })
    save_metrics(name, classifier, metrics, prf_by_label, conf_mx)
```

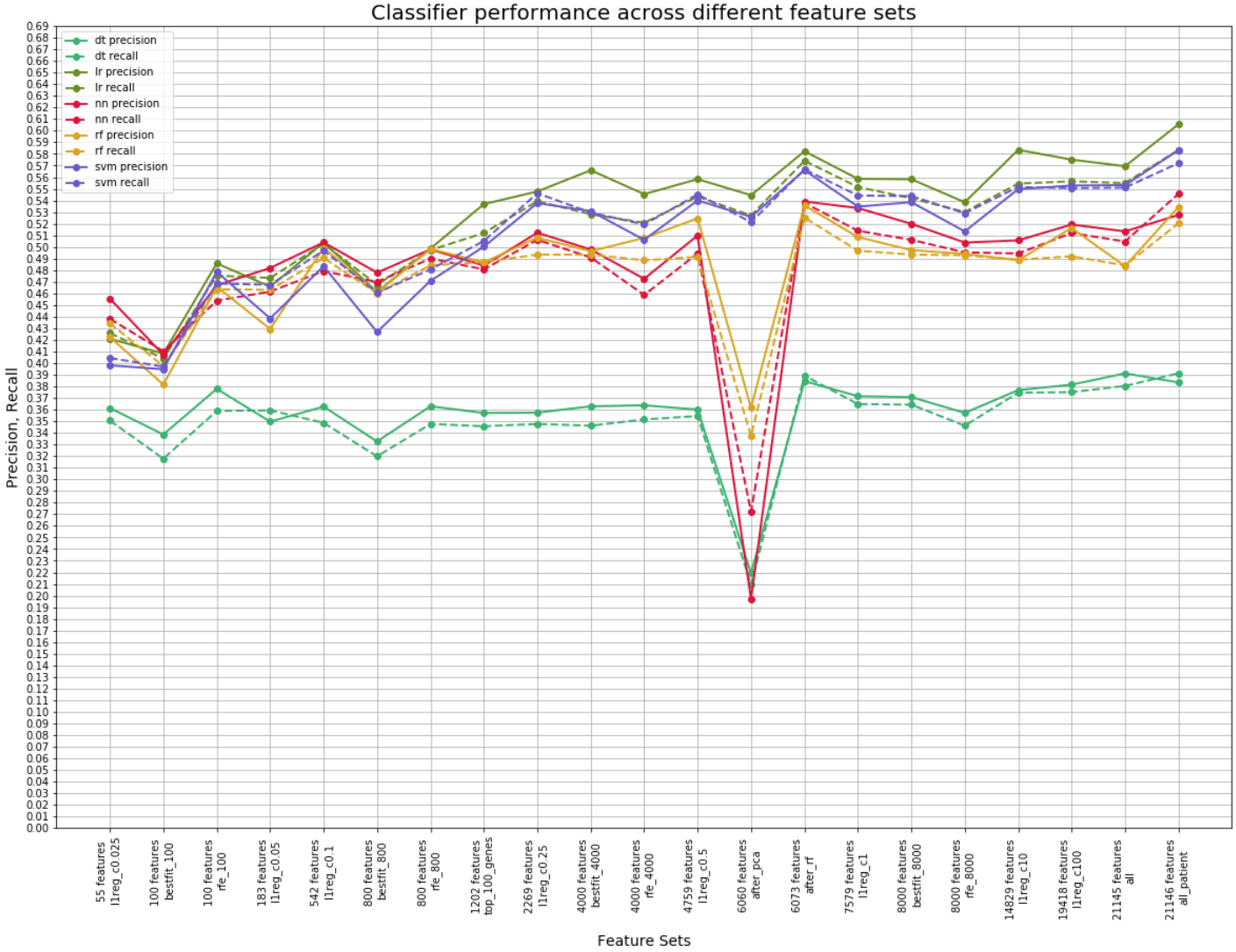
Load the metrics data

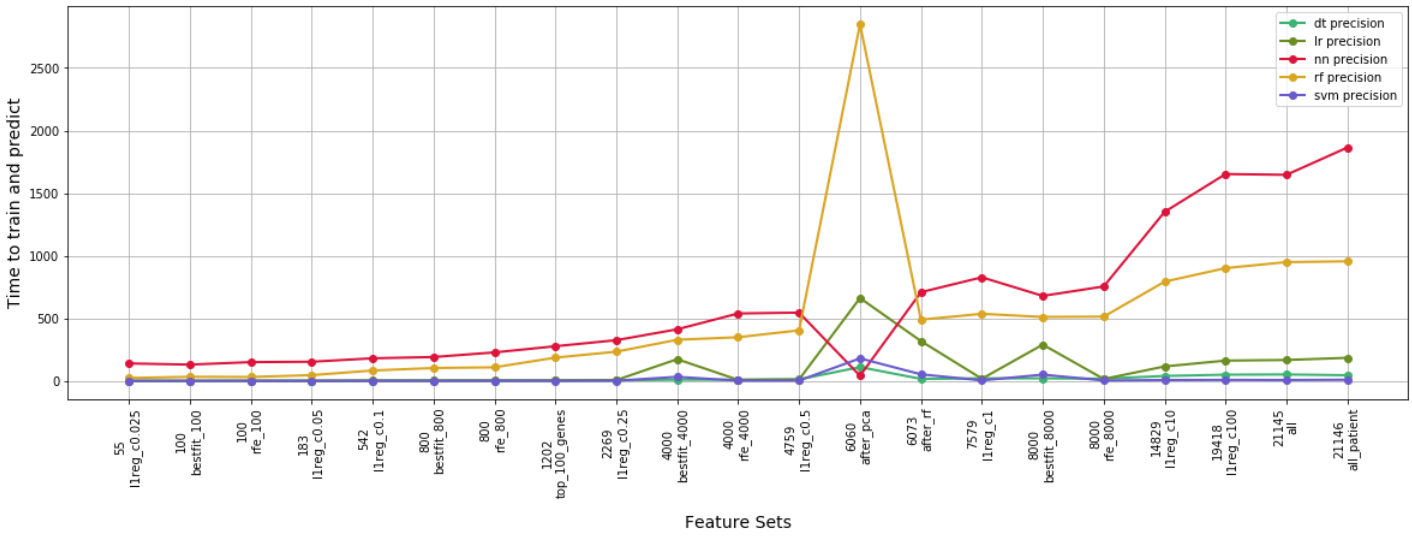
In [0]:
```
metrics_df = get_saved_metrics_dataframe()
metrics_df = metrics_df.sort_values(by=['feature_size', 'name', 'classifier'], ascending=[1,1,1])
metrics_df = metrics_df[metrics_df.columns[1:]]

metrics_df = metrics_df.sort_values(by=['classifier', 'feature_size', 'name'], ascending=[1,1,1])
```

In [0]:
```
colors = {'lr': 'olivedrab', 'svm': 'slateblue',
          'dt': 'mediumseagreen', 'rf': 'goldenrod',
          'xgb': 'coral', 'nn': 'crimson'}

def plot_classifier_metrics(metrics_df, label_encoder, description):

    plt.rcParams["figure.figsize"] = (20,14)

    labels = []
    for key, group in metrics_df.groupby(['feature_size', 'name']):
        labels.append(str(key[0]) + ' features \n' + key[1])


    sorted_df_report = metrics_df.sort_values(by=['classifier', 'feature_size', 'name'], ascending=[1,1,1])



    for classifier, group in sorted_df_report.groupby(['classifier']):

        plt.plot(labels, group.precision.values, color=colors[classifier],
                 linewidth=2, label=classifier + " precision", marker='o' )
        plt.plot(labels, group.recall.values, color=colors[classifier], linestyle="dashed",
                 linewidth=2, label=classifier + " recall", marker='o' )


    plt.yticks(np.arange(0, .70, .01))
    plt.title(description, fontsize=20)
    plt.ylabel('Precision, Recall', fontsize=14)
    plt.xlabel('Feature Sets', fontsize=14, labelpad=14)
    plt.xticks(rotation='vertical')
    plt.legend()
    plt.grid()
    plt.show()

    for classifier, group in sorted_df_report.groupby(['classifier']):

        plt.plot(labels, group.accuracy.values, color=colors[classifier],
                 linewidth=2, label=classifier + " accuracy", marker='o' )


    plt.yticks(np.arange(0, .70, .01))
    plt.ylabel('Accuracy', fontsize=14)
    plt.xticks(rotation='vertical')
    plt.xlabel('Features and Classifiers', fontsize=14, labelpad=20)
    plt.legend()
    plt.grid()
    plt.show()

def plot_classifier_times(metrics_df, label_encoder, description):

    plt.rcParams["figure.figsize"] = (20,6)

    labels = []
    for key, group in metrics_df.groupby(['feature_size', 'name']):
        labels.append(str(key[0]) + '\n' + key[1])

    sorted_df_report = metrics_df.sort_values(by=['classifier', 'feature_size', 'name'], ascending=[1,1,1])



    for classifier, group in sorted_df_report.groupby(['classifier']):

        plt.plot(labels, group.time.values, color=colors[classifier],
                 linewidth=2, label=classifier + " precision", marker='o' )



    plt.ylabel('Time to train and predict', fontsize=14)
    plt.xlabel('Feature Sets', fontsize=14, labelpad=14)
    plt.xticks(rotation='vertical')
    plt.legend()
    plt.grid()
    plt.show()



def coords_of_max(theArray, n):
    # Flatten the 2D array
    flat = theArray.flatten()
    # Partition so that the we know the sort order for
    # the cells with the highest values.  We just
    # care about the top n highest values.  So for example,
    # if n = 3, get return 3 indices.
    indices = np.argpartition(flat, -n)[-n:]
    # Reverse so that we show index of highest value first
    # (descending)
    indices = indices[np.argsort(-flat[indices])]
    # Now return the coordinates for these indices
    # for a 2D array.  This will return 2 arrays,
    # the first for the row index, the second for the
    # column index.  The row index represents the
    # actual digit, the column index represents
    # the confused digit
    return np.unravel_index(indices, theArray.shape)
```

Plot precision metrics across different classifiers and feature sets

In [0]:
```
label_encoder    = preprocessing.LabelEncoder()



# Plot precision, recall, accuracy across different classifiers
# for somatic mutations
plot_classifier_metrics(metrics_df, label_encoder, 'Classifier performance across different feature sets')

# Plot time across different classifiers
# for somatic mutations
plot_classifier_times(metrics_df, label_encoder, 'Time to train and run each model')
```


Classifier performance across different feature sets
dt precision
dt recall
lr precision
lr recall
nn precision
nn recall
rf precision
rf recall
svm precision
svm recall
Precision, Recall
Feature Sets
55 features l1reg_c0.025
100 features bestfit_100
100 features rfe_100
183 features l1reg_c0.05
542 features l1reg_c0.1
800 features bestfit_800
800 features rfe_800
1202 features top_100_genes
2269 features l1reg_c0.25
4000 features bestfit_4000
4000 features rfe_4000
4759 features l1reg_c0.5
6060 features after_pca
6073 features after_rf
7579 features l1reg_c1
8000 features bestfit_8000
8000 features rfe_8000
14829 features l1reg_c10
19418 features l1reg_c100
21145 features all
21146 features all_patient



Report the precision, recall, and f1 score across different classifiers and feature sets

In [0]:

```
def show_precision_recall_by_label(prf_by_label_df, name, classifier, label_encoder):

    plt.rcParams["figure.figsize"] = (16,14)

    labels = []
    for i in range(prf_by_label_df.shape[1]):
        label = label_encoder.inverse_transform([i])[0]
        labels.append(label)


    y_pos = np.arange(len(labels))

    fig, (ax1, ax2) = plt.subplots(ncols=2, sharey=False)

    ax1.invert_xaxis()
    ax1.invert_yaxis()
    ax1.yaxis.tick_right()

    ax1.set_yticks(y_pos)
    ax1.set_yticklabels(labels)

    ax2.invert_yaxis()
    ax2.set_yticks(y_pos)
    ax2.set_yticklabels(labels)

    ax1.barh(y_pos, prf_by_label_df.iloc[0].values, color=label_colors , label="precision")
    ax2.barh(y_pos, prf_by_label_df.iloc[1].values, color=label_colors,  label='recall')

    ax1.set_title('Precision( ' + classifier + ')')
    ax2.set_title('Recall (' + classifier + ')')
    ax1.grid()
    ax2.grid()


    plt.show()



# best precision
sorted_df = metrics_df.sort_values(by='precision', ascending=0)
best_precision = sorted_df.head(1)

# best recall
sorted_df = metrics_df.sort_values(by='recall', ascending=0)
best_recall = sorted_df.head(1)

# best f1
sorted_df = metrics_df.sort_values(by='f1', ascending=0)
best_f1 = sorted_df.head(1)

# best accuracy
sorted_df = metrics_df.sort_values(by='accuracy', ascending=0)
best_accuracy = sorted_df.head(1)


# Show the feature set and classifier with the best
# precision, recall, and f1 scores
print("\n\nBest precision")
display(best_precision)
print("\n\nBest recall")
display(best_recall)
print("\n\nBest f1")
display(best_f1)
print("\n\nBest accuracy")
display(best_accuracy)

# get the scores by label and confusion matrix
# for the best prediction
best_prediction = best_precision
best_name       = best_prediction.name.values[0]
best_classifier = best_prediction.classifier.values[0]


print("best name", best_name)

best_prf_by_label_df = get_prf_by_label(best_name, best_classifier)
best_confusion_mx_df = get_confusion_matrix(best_name, best_classifier)

feature_matrix = pd.read_csv("./data/features_" + best_name + ".train.csv")
label_encoder.fit(feature_matrix.cancer_type.unique())

# show a side-by-side barchart of precision and recall for each label
print("\n\nPrecision and Recall by Label with Best F1 score ")
print("Classifier:", best_classifier, "Feature set:", best_name)
show_precision_recall_by_label(best_prf_by_label_df,
                               best_name, best_classifier, label_encoder)
```

```
Best precision
```

	name	classifier	feature_size	accuracy	precision	recall	f1	time
65	all_patient	lr	21146	0.583374	0.605509	0.583374	0.556224	184.502283

```
Best recall
```

	name	classifier	feature_size	accuracy	precision	recall	f1	time
65	all_patient	lr	21146	0.583374	0.605509	0.583374	0.556224	184.502283

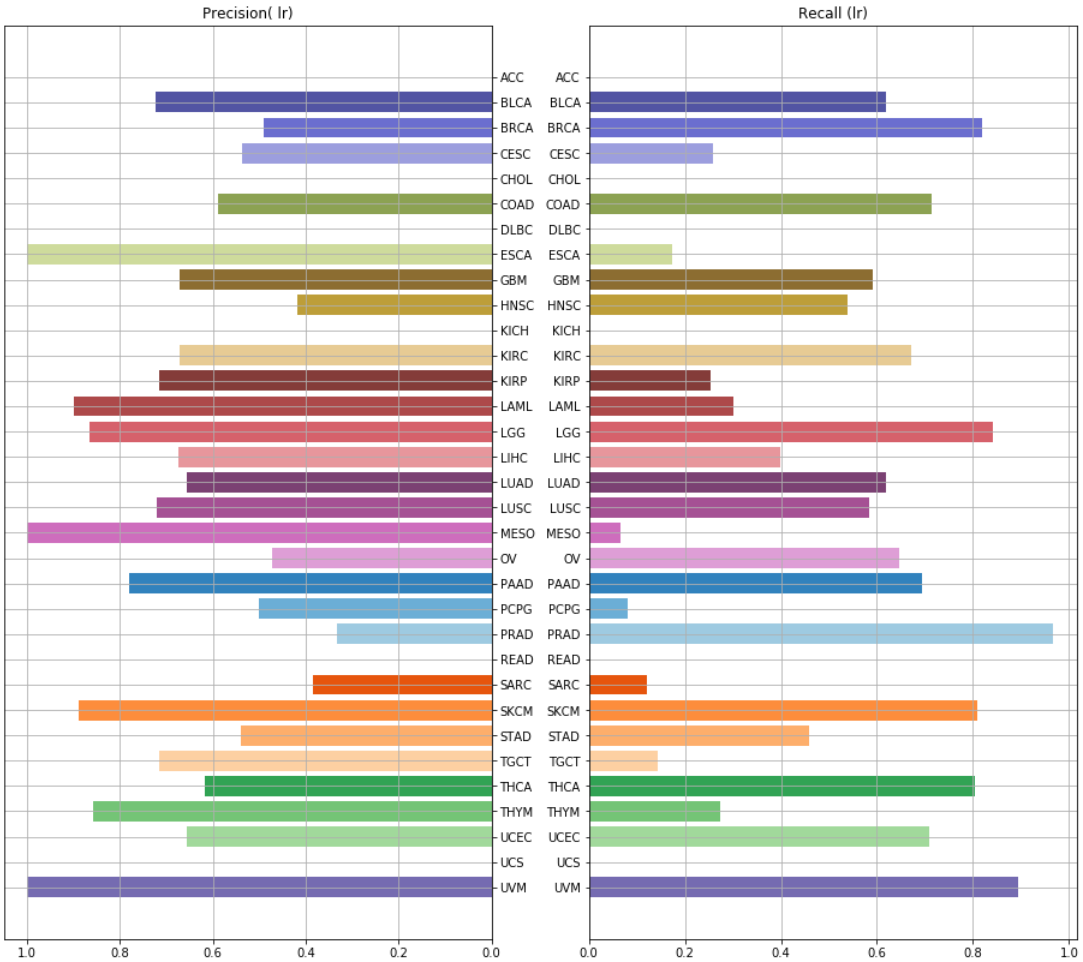
```
Best f1
```

	name	classifier	feature_size	accuracy	precision	recall	f1	time
65	all_patient	lr	21146	0.583374	0.605509	0.583374	0.556224	184.502283

```
Best accuracy
```

	name	classifier	feature_size	accuracy	precision	recall	f1	time
65	all_patient	lr	21146	0.583374	0.605509	0.583374	0.556224	184.502283

```
best name all_patient
Out[0]: LabelEncoder()

Precision and Recall by Label with Best F1 score
Classifier: lr Feature set: all_patient
```



The above bar charts showing precision and recall by label reveals that some of the cancer types have low prediction rates. In particular, cancer types ACC, CHOL, DLBC, KICH, READ, and UCS were not predicted for a single example in our test set. We observe that these are classes that have less < 150 cases, so this may partially explain low classifier performance. However, there are other cancer types with < 150 cases that have good precision and recall, specifically cancer type UVM. We will explore this discrepancy in predictions across classes in the the sections below as well as notebook 05.

Visualizations for Diagnosing Poor Performing Classes

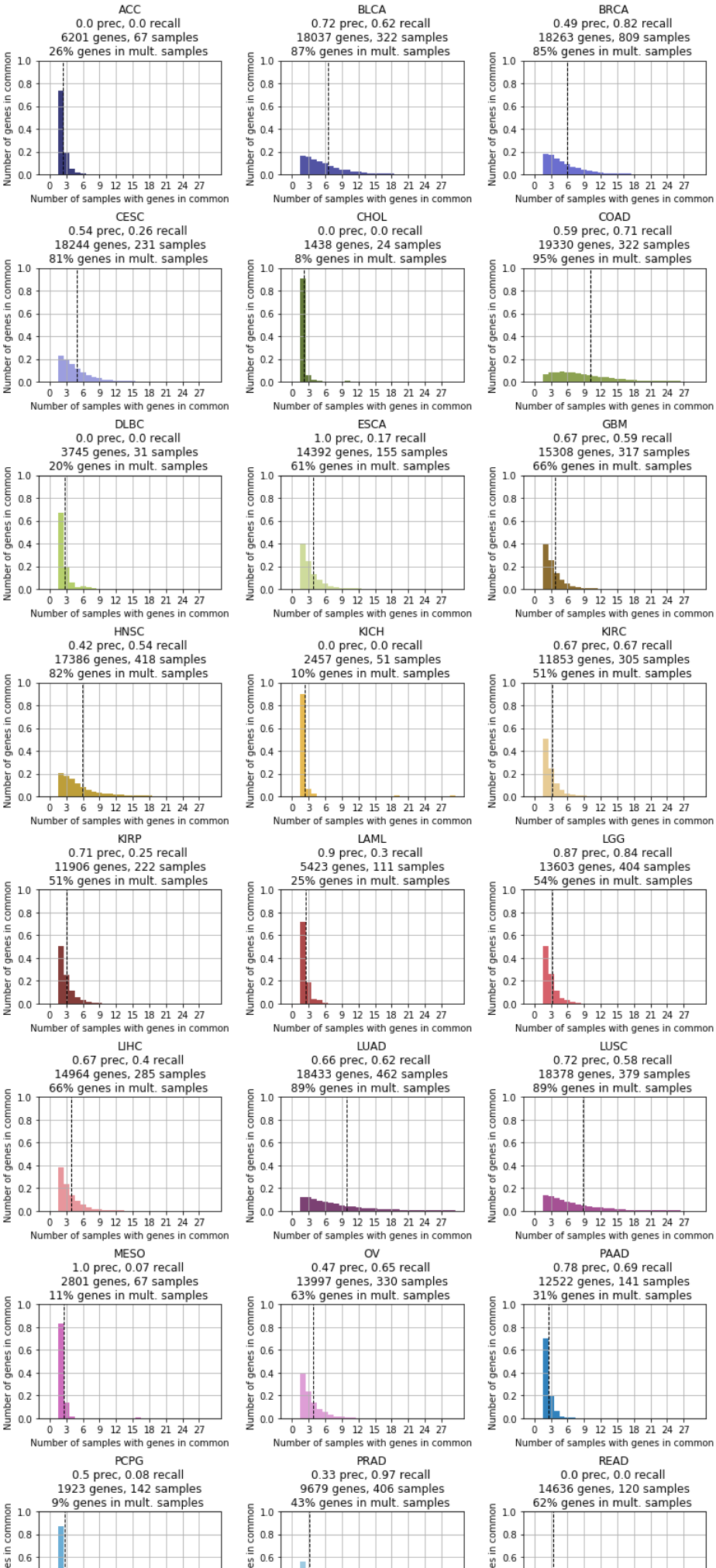
How many genes are in common for a cancer type?

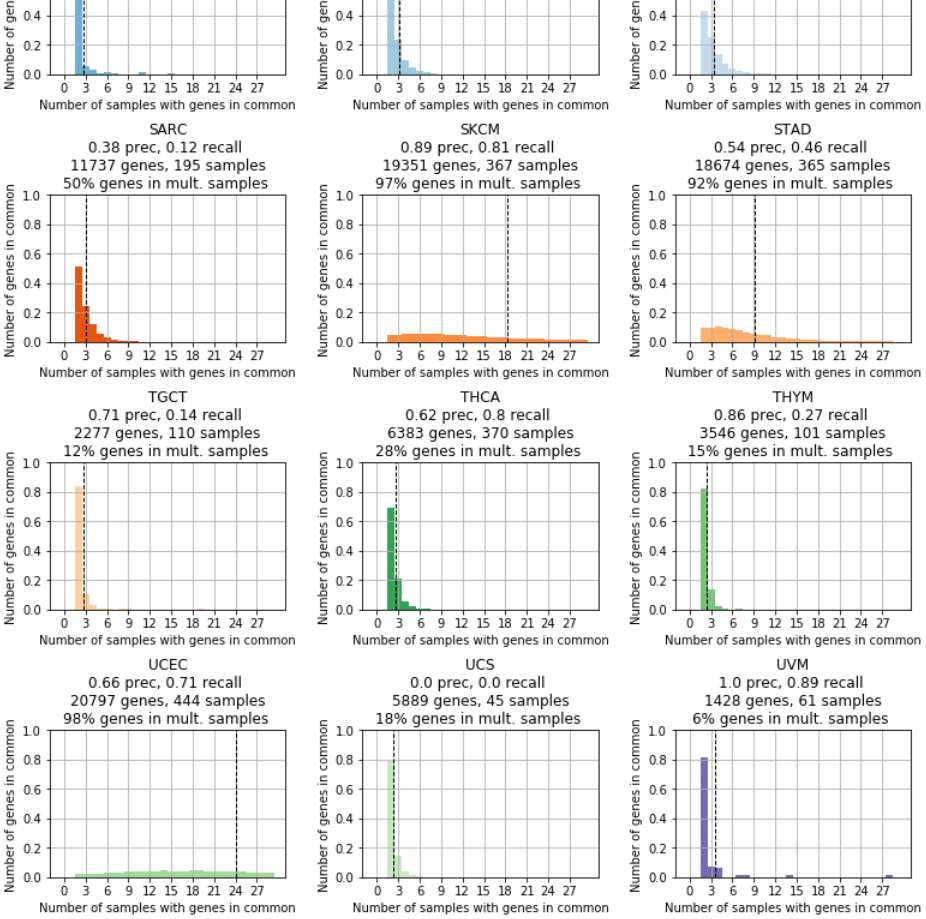
In [0]:

```
features       = feature_matrix[feature_matrix.columns[1:]]
cancer_types   = sorted(features.cancer_type.unique())
best_precision = np.round(best_prf_by_label_df.iloc[0],2)
best_recall    = np.round(best_prf_by_label_df.iloc[1],2)

plt.rcParams["figure.figsize"] = (11,35)
fig = plt.figure()
suptitle = fig.suptitle("Number of Genes in Common for Samples of a Cancer Type", fontsize=20)
ax = fig.subplots(11, 3, sharex=False, sharey=False, squeeze=True)
plt.subplots_adjust(hspace=0.4)
ax = ax.flatten()

num_samples_per_cancer_type = []
num_genes_per_cancer_type   = []
num_multisample_genes_per_cancer_type = []
pct_multisample_genes_per_cancer_type = []
avg_num_samples_sharing_genes = []


for idx, cancer_type in enumerate(cancer_types, start=0):
  features_ct = features.loc[features.cancer_type == cancer_type]
  features_ct = features_ct[features_ct.columns[2:]]

  print(".", end='')


  gene_sums_all = features_ct.sum(axis=0)
  gene_sums_all = gene_sums_all[gene_sums_all > 0]
  gene_sums = gene_sums_all[gene_sums_all > 1]
  gene_sums.columns = ['gene_count']


  num_samples_per_cancer_type.append(features_ct.shape[0])
  num_genes_per_cancer_type.append(gene_sums_all.shape[0])
  num_multisample_genes_per_cancer_type.append(gene_sums.shape[0])
  pct_multisample_genes_per_cancer_type.append((gene_sums.shape[0] / gene_sums_all.shape[0]) * 100)
  avg_num_samples_sharing_genes.append(gene_sums.mean(axis=0))

  bins = np.arange(31) - 0.5
  _ = gene_sums.hist(ax=ax[idx], bins=bins, density=True, range=[0,31], color=label_colors[idx] )
  _ = ax[idx].set_title(cancer_type + "\n"
                        + str(best_precision[idx]) + " prec, " + str(best_recall[idx]) + " recall \n"
                        + str(gene_sums_all.shape[0]) + " genes, " + str(features_ct.shape[0]) + " samples\n"
                        + str(int(np.round(gene_sums.shape[0] / gene_sums_all.shape[0], 2) * 100)) + "% genes in mult. samples ")

  _ = ax[idx].axvline(gene_sums.mean(), color='k', linestyle='dashed', linewidth=1)
  _ = ax[idx].set_xlabel("Number of samples with genes in common")
  _ = ax[idx].set_ylim((0,1))
  _ = ax[idx].set_xticks(np.arange(0, 30, 3))
  _ = ax[idx].set_ylabel("Number of genes in common")

_ = fig.tight_layout()
_ = suptitle.set_y(1)
_ = fig.subplots_adjust(top=.95)
plt.show()
```

.....

Number of Genes in Common for Samples of a Cancer Type





In the plots above, we show if mutated genes for a cancer type are shared across the patient sample tumors. We assume that the more common a gene mutation appears across cases of the same cancer type, the better predictive power.

Here we two distinct distributions. For most of the low predicted cancer types, we see the heavy left skewed distribution, with only a few genes common across the cases. These include the following cancer types, all with < 150 cases: ACC, CHOL, DLBC, KICH, READ, and UCS.

The second distribution we see is a flatter, has a higher mean, and is spread across a broader range. In general, these are cancer types yield better predictions, which corresponds to our assumption that gene mutations common across cases of a given cancer type will have more predictive power. Note that these are the cancer types that have more examples. Again, we see that UVM is an exception to this case.

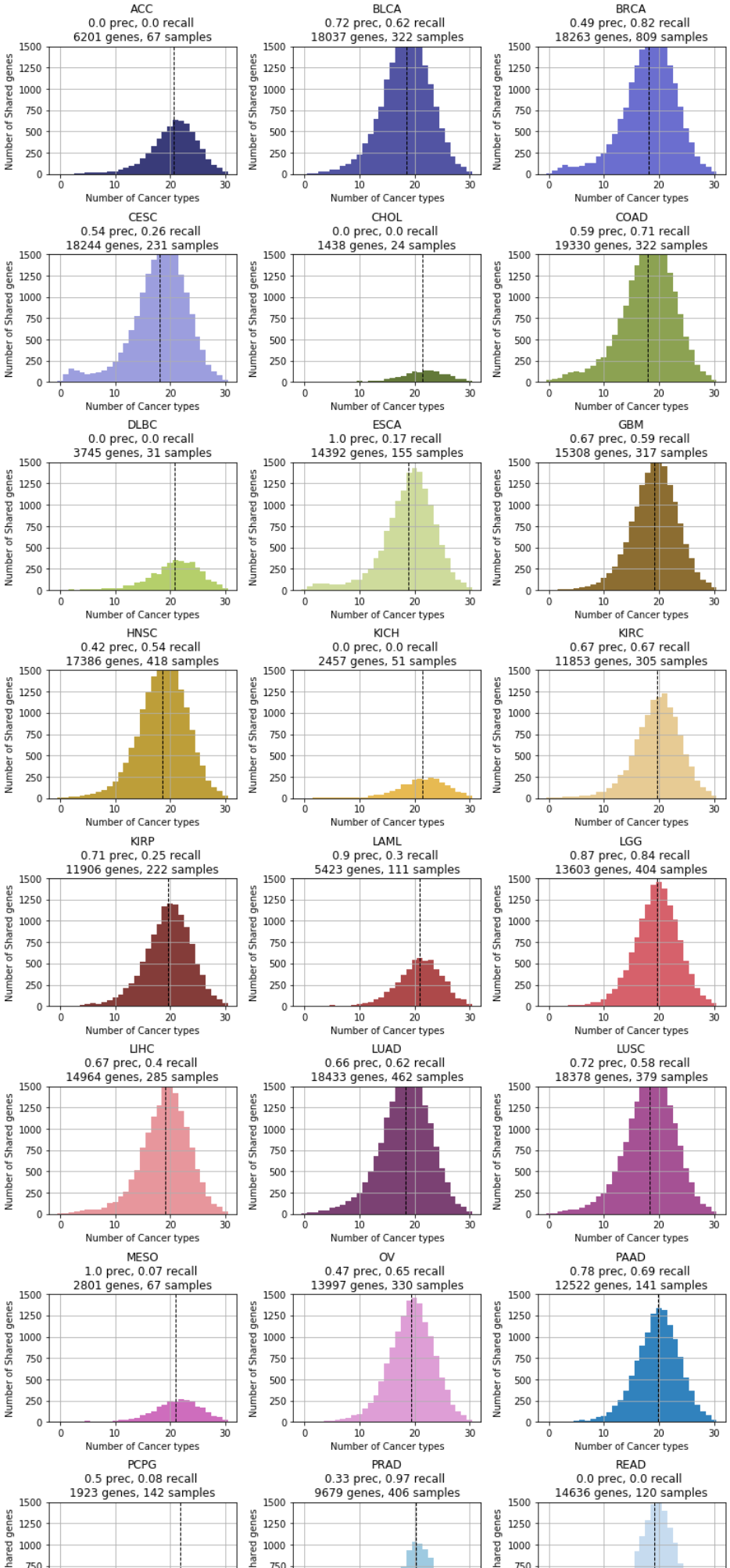
How many genes are common across all cancer types?

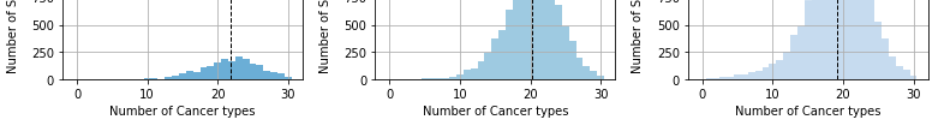
In [0]:

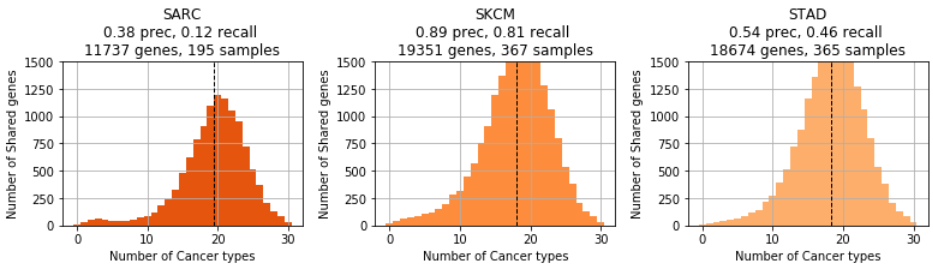
```
plt.rcParams["figure.figsize"] = (11,35)
fig = plt.figure()
suptitle = fig.suptitle("Number of Genes for a Cancer Type that are common across other Cancer Types", fontsize=20)
ax = fig.subplots(11, 3, sharex=False, sharey=False, squeeze=True)
_ = plt.subplots_adjust(hspace=0.4)
ax = ax.flatten()

mean_common_cancer_types = []

features_by_cc = features[features.columns[1:]].groupby(['cancer_type']).sum()
for col in features_by_cc.columns:
  features_by_cc[col] = features_by_cc[col].apply(lambda x: 0 if x == 0 else 1)


diff_pairings = []

for idx, cancer_type in enumerate(cancer_types, start=0):
  print(".", end='')
  features_ct = features_by_cc.loc[[cancer_type]]

  gene_counts_ct = features_ct.T
  non_zero_genes = list(gene_counts_ct[gene_counts_ct[cancer_type] > 0].index)

  other_cancer_types = [c for c in cancer_types if c != cancer_type]
  features_other = features_by_cc.loc[other_cancer_types, non_zero_genes]

  gene_sums_ct = features_ct.sum(axis=0)
  gene_sums_ct = gene_sums_ct[gene_sums_ct > 0]
  gene_sums_ct.columns = ['gene_count']

  gene_sums_other = features_other.sum(axis=0)
  gene_sums_other = gene_sums_other[gene_sums_ct > 0]
  gene_sums_other.columns = ['gene_count']

  sums_other     = features_other.sum(axis=0)

  mean_common_cancer_types.append(sums_other.mean())


  diff_pairing       = []
  diff_pairing_norm  = []
  for x, cancer_type_pairing in enumerate(cancer_types, start=0):
    features_pairing    = features_by_cc.loc[[cancer_type_pairing]]
    gene_counts_pairing = features_pairing.T
    non_zero_target     = set(non_zero_genes)
    non_zero_other      = list(gene_counts_pairing[gene_counts_pairing[cancer_type_pairing] > 0].index)
    non_zero_other      = set(non_zero_other)

    diff = non_zero_target - non_zero_other

    diff_pairing.append(len(diff))

  diff_pairings.append(diff_pairing)

  bins = np.arange(32) - 0.5
  _ = sums_other.hist(ax=ax[idx], bins=bins, range=[0,33], color=label_colors[idx])
  _ = ax[idx].set_ylim((0,1500))
  _ = ax[idx].axvline(sums_other.mean(), color='k', linestyle='dashed', linewidth=1)
  _ = ax[idx].set_title(cancer_type + " (" + str(gene_sums_ct.shape[0]) + " genes, "
                        + "prec=" + str(best_precision[idx]) + ")")

  _ = ax[idx].set_title(cancer_type + "\n"
                        + str(best_precision[idx]) + " prec, " + str(best_recall[idx]) + " recall \n"
                        + str(gene_sums_ct.shape[0]) + " genes, " + str(num_samples_per_cancer_type[idx]) + " samples")

  _ = ax[idx].set_xlabel("Number of Cancer types")
  _ = ax[idx].set_ylabel("Number of Shared genes")


fig.tight_layout()
suptitle.set_y(1)
fig.subplots_adjust(top=.95)
plt.show()
```

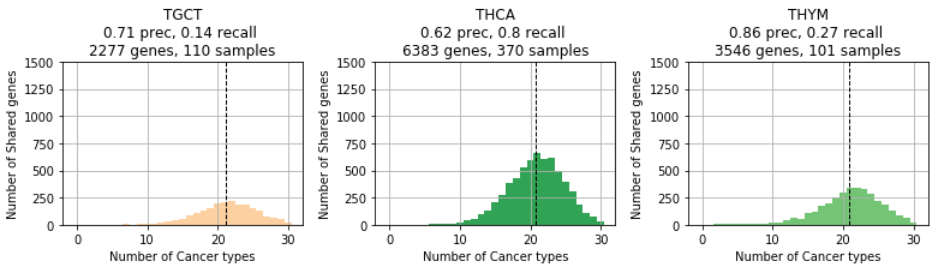
.....

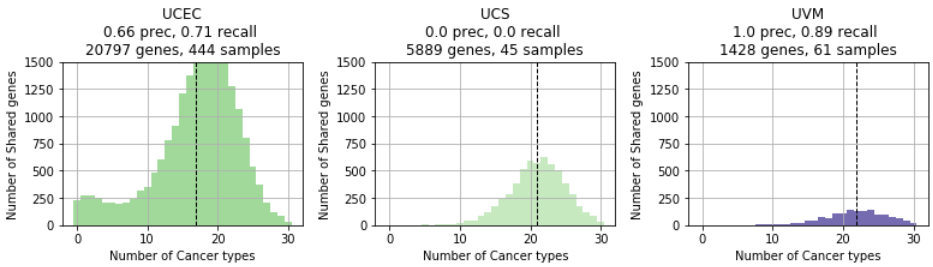
Number of Genes for a Cancer Type that are common across other Cancer Types





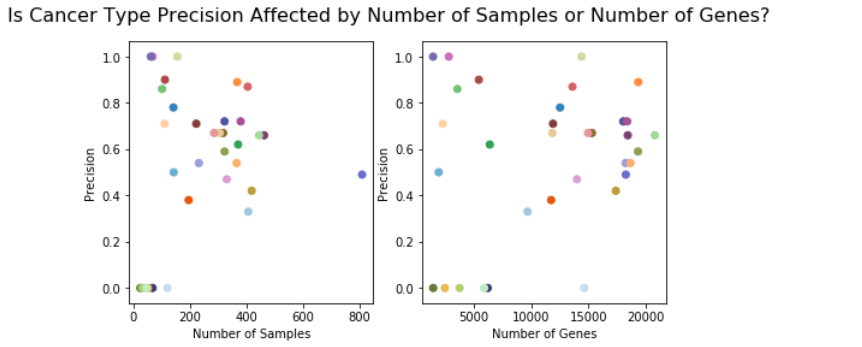


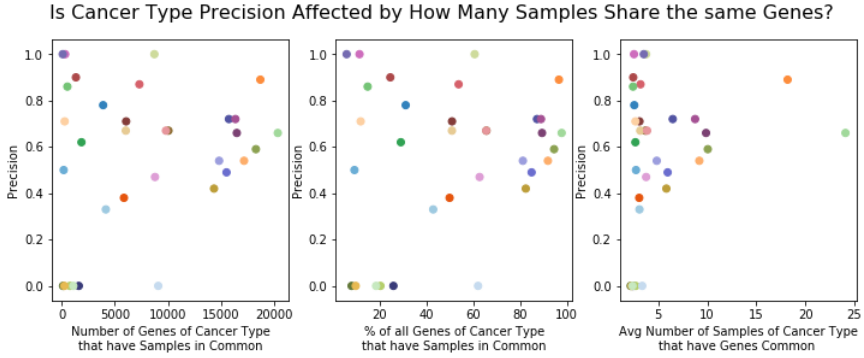


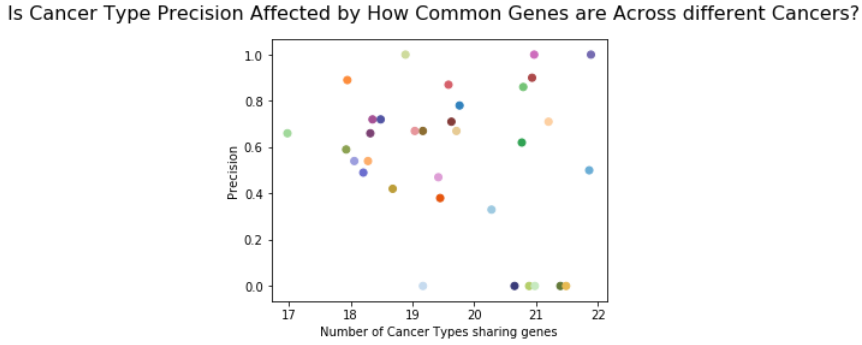


In the plots above, we try a different approach, looking at the number of genes for a cancer type that are common across the other cancer types. Here, we want to see if the lower performing classes have a different distribution or mean. However, we can see that across all cancer types, many of the genes are in common.

In [0]:
```
plt.rcParams["figure.figsize"] = (8,4)
fig = plt.figure()
suptitle = fig.suptitle("Is Cancer Type Precision Affected by Number of Samples or Number of Genes?",
                        fontsize=16)
ax = fig.subplots(1, 2, sharex=False, sharey=False, squeeze=True)

_ = ax[0].scatter(num_samples_per_cancer_type, best_precision, color=label_colors)
_ = ax[0].set_ylabel("Precision")
_ = ax[0].set_xlabel("Number of Samples")

_ = ax[1].scatter(num_genes_per_cancer_type, best_precision, color=label_colors)
_ = ax[1].set_ylabel("Precision")
_ = ax[1].set_xlabel("Number of Genes")


plt.rcParams["figure.figsize"] = (12,4)
fig = plt.figure()
suptitle = fig.suptitle("Is Cancer Type Precision Affected by How Many Samples Share the same Genes?",
                        fontsize=16)
ax = fig.subplots(1, 3, sharex=False, sharey=False, squeeze=True)

_ = ax[0].scatter(num_multisample_genes_per_cancer_type, best_precision, color=label_colors)
_ = ax[0].set_ylabel("Precision")
_ = ax[0].set_xlabel("Number of Genes of Cancer Type\nthat have Samples in Common")


_ = ax[1].scatter(pct_multisample_genes_per_cancer_type , best_precision, color=label_colors)
_ = ax[1].set_ylabel("Precision")
_ = ax[1].set_xlabel("% of all Genes of Cancer Type\nthat have Samples in Common")


_ = ax[2].scatter(avg_num_samples_sharing_genes, best_precision, color=label_colors)
_ = ax[2].set_ylabel("Precision")
_ = ax[2].set_xlabel("Avg Number of Samples of Cancer Type\nthat have Genes Common ")



plt.rcParams["figure.figsize"] = (5,4)
fig = plt.figure()
suptitle = fig.suptitle("Is Cancer Type Precision Affected by How Common Genes are Across different Cancers?",
                        fontsize=16)
ax = fig.subplots(1, 1, sharex=False, sharey=False, squeeze=True)

_ = ax.scatter(mean_common_cancer_types, best_precision, color=label_colors)
_ = ax.set_ylabel("Precision")
_ = ax.set_xlabel("Number of Cancer Types sharing genes")
```





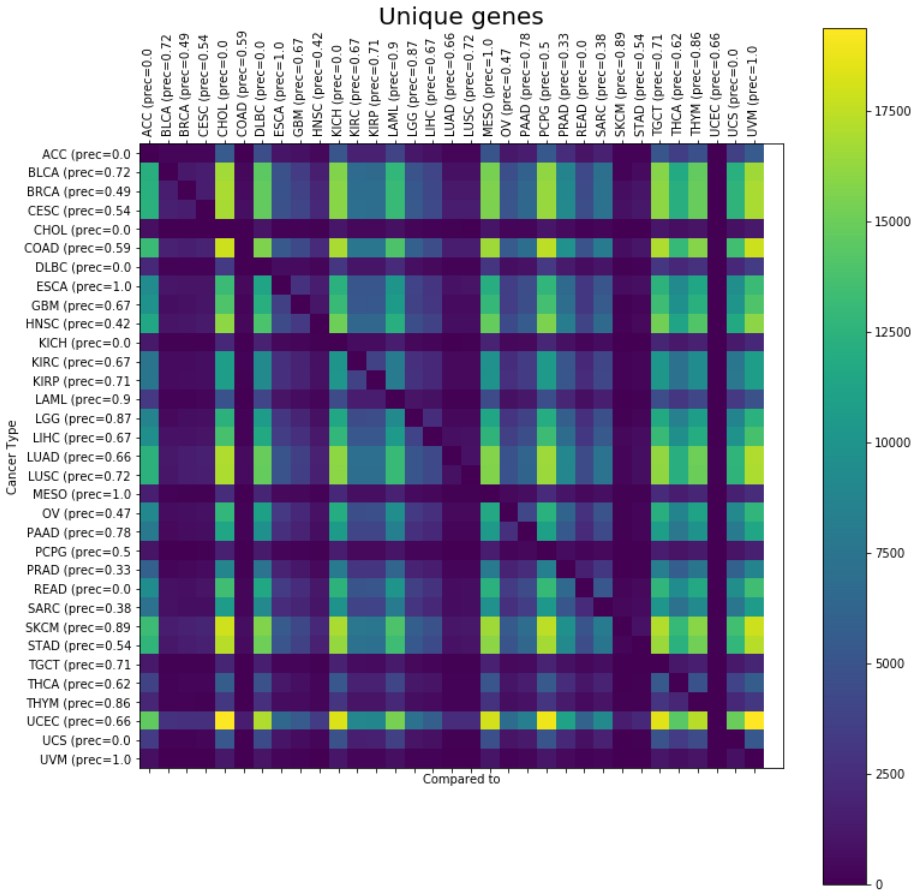


In the above scatter plots, we look for any correlation between precision and other factors, like number of samples, number of genes (first row of plots). There appears to be no strong correlation, so it is unclear that adding more examples of the cancer types would improve the predictions.

The second row of plots explores the number of genes in common in the cases for a cancer type and looks for any correlation to precision. Again, no clear correlation appears, although the same outliers in the upper left corner appear.

Pairwise comparison of cancer types, how unique is the set of genes for each cancer type?

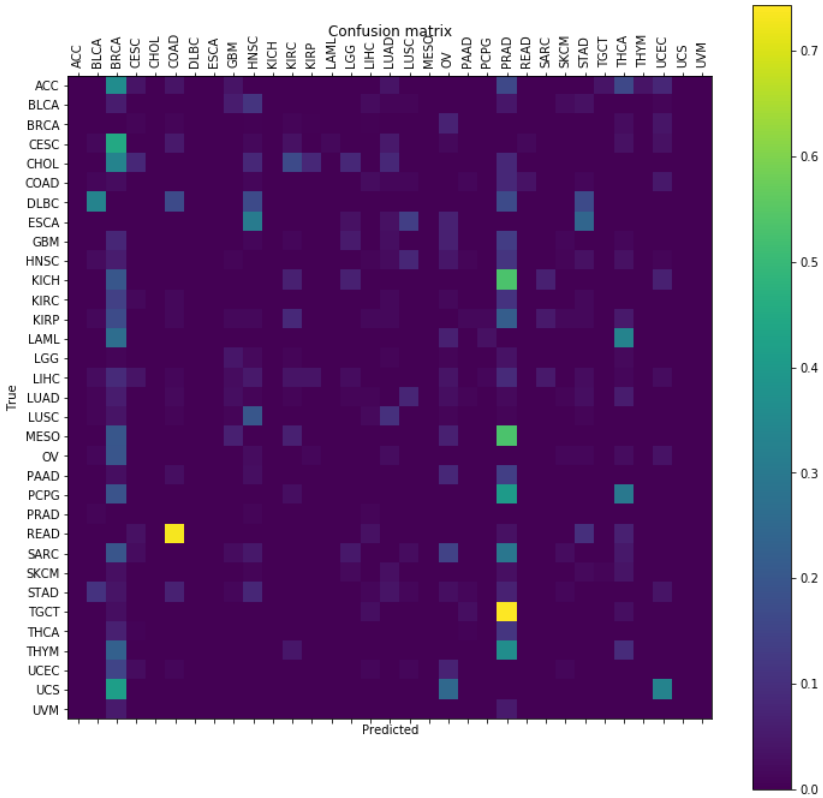
In [0]:
```
informative_labels = []
for i in range(len(cancer_types)):
  informative_labels.append(cancer_types[i] + " (prec=" + str(best_precision[i]))

def plot_pairwise_comparison(pairings, title):

  pairing_df = pd.DataFrame(pairings, columns=informative_labels, index=informative_labels)
  pairing_df['precision'] = best_precision

  plt.rcParams["figure.figsize"] = (12,12)
  fig = plt.figure()
  ax = fig.add_subplot(111)
  cax = ax.matshow(pairing_df)
  the_title = plt.title(title, fontsize=20)
  _ = fig.colorbar(cax)
  _ = ax.set_xticks(np.arange(0, 33, 1.0))
  _ = ax.set_yticks(np.arange(0, 33, 1.0))
  _ = ax.set_xticklabels(informative_labels, rotation='vertical')
  _ = ax.set_yticklabels(informative_labels)
  _ = plt.xlabel('Compared to')
  _ = plt.ylabel('Cancer Type')
  _ = the_title.set_y(1.18)
  _ = fig.subplots_adjust(top=.95)
  plt.show()

plot_pairwise_comparison(diff_pairings, "Unique genes")
```



In the matrix above we explore if there is a unique set of genes that sets apart one cancer type from another. The chart should read row by row. Each row represents a cancer type. The columns are brighter when the cancer type in the row has a higher number of unique genes from the cancer type in the column. So in general, we look for rows that are dark, indicating there is no unique gene set that characterizes the cancer type. Again, our lower performing classes with low number of examples, show up as dark blue rows, (e.g. ACC, CHOL, DLBC, KICH, READ, and UCS). Note also, that cancer types with higher precision have brighter rows (e.g. SKCM, BLCA, LUSC).

Show the confusion matrix for the best performing classifier/feature set

In [0]:
```
def show_confusion_matrix(conf_mx, label_encoder):


    # Determine the error rates for each misclassification pair
    row_sums = conf_mx.sum(axis=1, keepdims=True)
    norm_conf_mx = conf_mx / row_sums
    # Set the error rates for correctly classified pairs (the diagonal) to zero
    np.fill_diagonal(norm_conf_mx, 0)


    plt.rcParams["figure.figsize"] = (12,12)
    fig = plt.figure()
    ax = fig.add_subplot(111)
    cax = ax.matshow(norm_conf_mx)
    _ = plt.title('Confusion matrix')
    _ = fig.colorbar(cax)
    _ = ax.set_xticks(np.arange(0, 33, 1.0))
    _ = ax.set_yticks(np.arange(0, 33, 1.0))
    _ = ax.set_xticklabels(cancer_types, rotation='vertical')
    _ = ax.set_yticklabels(cancer_types)
    _ = plt.xlabel('Predicted')
    _ = plt.ylabel('True')
    plt.show()

    max_coords = coords_of_max(norm_conf_mx, 50)
    confusion_rows = []
    for i in range(len(max_coords[0])):

        # This is the actual label
        actual_label_idx  = max_coords[0][i]
        actual_label      = label_encoder.inverse_transform([actual_label_idx])[0]

        # This is the predicted label
        predicted_label_idx = max_coords[1][i]
        predicted_label = label_encoder.inverse_transform([predicted_label_idx])[0]

        # This is the error rate
        error_rate  = norm_conf_mx[max_coords[0][i], max_coords[1][i]]
        error_count = conf_mx[max_coords[0][i], max_coords[1][i]]

        row = list([ actual_label,
                     predicted_label,
                     code_to_disease[actual_label][0],
                     code_to_disease[predicted_label][0],
                     error_rate,
                     error_count ])
        confusion_rows.append(row)

    df = pd.DataFrame(confusion_rows, columns=['actual', 'predicted',  'actual_name', 'predicted_name', 'error_rate', 'error_count'])
    display(df)


cols = [c for c in best_confusion_mx_df.columns]
best_confusion_mx = best_confusion_mx_df[cols].values
show_confusion_matrix(best_confusion_mx, label_encoder)
```


Confusion matrix
ACC
BLCA
BRCA
CESC
CHOL
COAD
DLBC
ESCA
GBM
HNSC
KICH
KIRC
KIRP
LAML
LGG
LIHC
LUAD
LUSC
MESO
OV
PAAD
PCPG
PRAD
READ
SARC
SKCM
STAD
TGCT
THCA
THYM
UCEC
UCS
UVM
True
Predicted
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

	actual	predicted	actual_name	predicted_name	error_rate	error_count
0	TGCT	PRAD	Testicular_Germ_Cell_Tumors	Prostate_adenocarcinoma	0.742857	26
1	READ	COAD	Rectum_adenocarcinoma	Colon_adenocarcinoma	0.733333	22
2	KICH	PRAD	Kidney_Chromophobe	Prostate_adenocarcinoma	0.533333	8
3	MESO	PRAD	Mesothelioma	Prostate_adenocarcinoma	0.533333	8
4	CESC	BRCA	Cervical_squamous_cell_carcinoma_and_endocervi...	Breast_invasive_carcinoma	0.448276	26
5	UCS	BRCA	Uterine_Carcinosarcoma	Breast_invasive_carcinoma	0.416667	5
6	PCPG	PRAD	Pheochromocytoma_and_Paraganglioma	Prostate_adenocarcinoma	0.405405	15
7	THYM	PRAD	Thymoma	Prostate_adenocarcinoma	0.363636	8
8	ACC	BRCA	Adrenocortical_carcinoma	Breast_invasive_carcinoma	0.360000	9
9	UCS	UCEC	Uterine_Carcinosarcoma	Uterine_Corpus_Endometrial_Carcinoma	0.333333	4
10	CHOL	BRCA	Cholangiocarcinoma	Breast_invasive_carcinoma	0.333333	4
11	LAML	THCA	Acute_Myeloid_Leukemia	Thyroid_carcinoma	0.333333	10
12	DLBC	BLCA	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Bladder_Urothelial_Carcinoma	0.333333	2
13	ESCA	HNSC	Esophageal_carcinoma	Head_and_Neck_squamous_cell_carcinoma	0.310345	9
14	PCPG	THCA	Pheochromocytoma_and_Paraganglioma	Thyroid_carcinoma	0.297297	11
15	SARC	PRAD	Sarcoma	Prostate_adenocarcinoma	0.292683	12
16	LAML	BRCA	Acute_Myeloid_Leukemia	Breast_invasive_carcinoma	0.266667	8
17	UCS	OV	Uterine_Carcinosarcoma	Ovarian_serous_cystadenocarcinoma	0.250000	3
18	ESCA	STAD	Esophageal_carcinoma	Stomach_adenocarcinoma	0.241379	7
19	THYM	BRCA	Thymoma	Breast_invasive_carcinoma	0.227273	5
20	KIRP	PRAD	Kidney_renal_papillary_cell_carcinoma	Prostate_adenocarcinoma	0.220339	13
21	MESO	BRCA	Mesothelioma	Breast_invasive_carcinoma	0.200000	3
22	KICH	BRCA	Kidney_Chromophobe	Breast_invasive_carcinoma	0.200000	3
23	LUSC	HNSC	Lung_squamous_cell_carcinoma	Head_and_Neck_squamous_cell_carcinoma	0.198113	21
24	SARC	BRCA	Sarcoma	Breast_invasive_carcinoma	0.195122	8
25	OV	BRCA	Ovarian_serous_cystadenocarcinoma	Breast_invasive_carcinoma	0.195122	16
26	PCPG	BRCA	Pheochromocytoma_and_Paraganglioma	Breast_invasive_carcinoma	0.189189	7
27	KIRP	BRCA	Kidney_renal_papillary_cell_carcinoma	Breast_invasive_carcinoma	0.169492	10
28	DLBC	HNSC	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Head_and_Neck_squamous_cell_carcinoma	0.166667	1
29	DLBC	STAD	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Stomach_adenocarcinoma	0.166667	1
30	DLBC	PRAD	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Prostate_adenocarcinoma	0.166667	1
31	DLBC	COAD	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Colon_adenocarcinoma	0.166667	1
32	CHOL	KIRC	Cholangiocarcinoma	Kidney_renal_clear_cell_carcinoma	0.166667	2
33	ACC	THCA	Adrenocortical_carcinoma	Thyroid_carcinoma	0.160000	4
34	ACC	PRAD	Adrenocortical_carcinoma	Prostate_adenocarcinoma	0.160000	4
35	UCEC	BRCA	Uterine_Corpus_Endometrial_Carcinoma	Breast_invasive_carcinoma	0.151163	13
36	SARC	OV	Sarcoma	Ovarian_serous_cystadenocarcinoma	0.146341	6
37	KIRC	BRCA	Kidney_renal_clear_cell_carcinoma	Breast_invasive_carcinoma	0.140625	9
38	PAAD	PRAD	Pancreatic_adenocarcinoma	Prostate_adenocarcinoma	0.138889	5
39	ESCA	LUSC	Esophageal_carcinoma	Lung_squamous_cell_carcinoma	0.137931	4
40	GBM	PRAD	Glioblastoma_multiforme	Prostate_adenocarcinoma	0.131579	10
41	THCA	PRAD	Thyroid_carcinoma	Prostate_adenocarcinoma	0.114754	14
42	BLCA	HNSC	Bladder_Urothelial_Carcinoma	Head_and_Neck_squamous_cell_carcinoma	0.112360	10
43	HNSC	PRAD	Head_and_Neck_squamous_cell_carcinoma	Prostate_adenocarcinoma	0.112360	10
44	KIRC	PRAD	Kidney_renal_clear_cell_carcinoma	Prostate_adenocarcinoma	0.109375	7
45	STAD	BLCA	Stomach_adenocarcinoma	Bladder_Urothelial_Carcinoma	0.108108	8
46	LUSC	LUAD	Lung_squamous_cell_carcinoma	Lung_adenocarcinoma	0.103774	11
47	READ	STAD	Rectum_adenocarcinoma	Stomach_adenocarcinoma	0.100000	3
48	THYM	THCA	Thymoma	Thyroid_carcinoma	0.090909	2
49	LIHC	BRCA	Liver_hepatocellular_carcinoma	Breast_invasive_carcinoma	0.089744	7

Finally, we show a normalized confusion matrix in plot form. The brighter cells represent a higher error rate where the cancer type in the row (true) is being misclassified as the cancer type in the column (predicted). Here we notice two classes (columns) that appear to be predicted in error across many cancer types; BRCA and PRAD. Incorrect BRCA (Breast invasive carcinoma) predictions are most likely due to an unbalanced classification -- this cancer type has over 800 of the cases in the dataset. PRAD (Prostate adenocarcinoma) is often misclassified as TGCT (Testicular Germ Cell Tumors). Similarly, COAD (Colon_adenocarcinoma) is ofen misclassified as READ (Rectum_adenocarcinoma). I

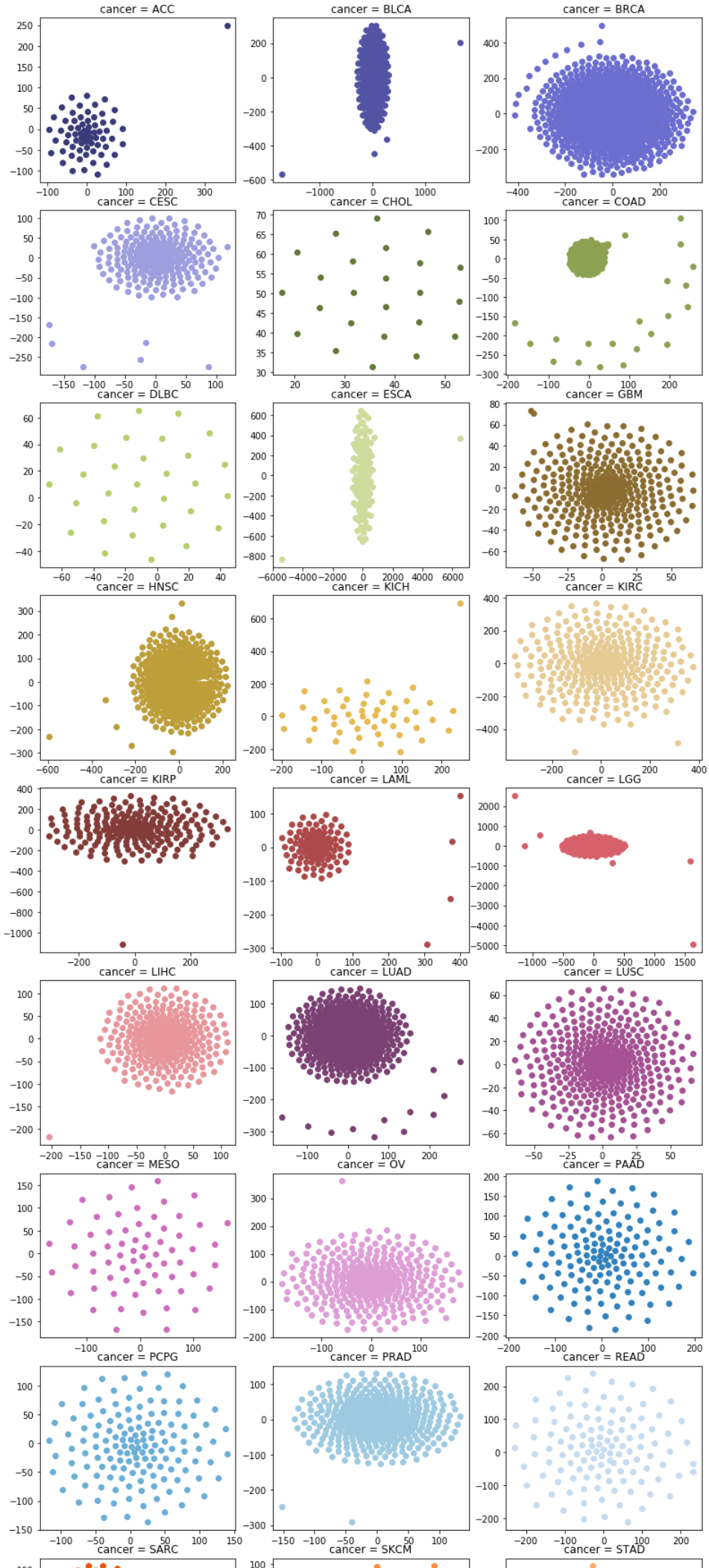
TSNE Visualization

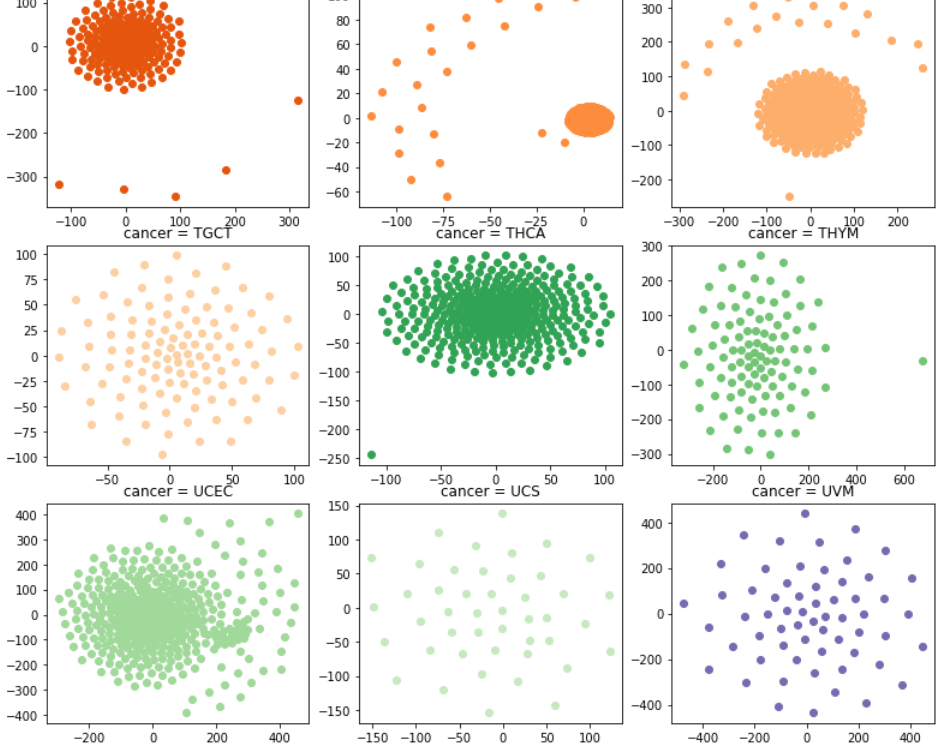
In [0]:

```
from sklearn.manifold import TSNE
import matplotlib as mpl

label_encoder   = preprocessing.LabelEncoder()

labels  = list(feature_matrix.cancer_type.unique())
labels.sort()
X       = feature_matrix[feature_matrix.columns[3:]]
label_encoder.fit(labels)

print("Plot TSNE...")
N = len(labels)
colors = mpl.cm.rainbow(np.linspace(0, 1, N))
fig, axes = plt.subplots(nrows=11, ncols=3, figsize=(11, 33))
_ = plt.tight_layout()

for i, ax in enumerate(axes.flat):
    if (i < len(labels)):
      ax.title.set_text("cancer = {}".format(labels[i]))
      d = X[feature_matrix['cancer_type'] == labels[i]]
      dd = TSNE(n_components=2).fit_transform(d)
      _ = ax.scatter(dd[:,0], dd[:,1], color=label_colors[i])
plt.show()
```

Out[0]: LabelEncoder()

Plot TSNE...


cancer = ACC
cancer = BLCA
cancer = BRCA
cancer = CESC
cancer = CHOL
cancer = COAD
cancer = DLBC
cancer = ESCA
cancer = GBM
cancer = HNSC
cancer = KICH
cancer = KIRC
cancer = KIRP
cancer = LAML
cancer = LGG
cancer = LIHC
cancer = LUAD
cancer = LUSC
cancer = MESO
cancer = OV
cancer = PAAD
cancer = PCPG
cancer = PRAD
cancer = READ
cancer = SARC
cancer = SKCM
cancer = STAD



TSNE (T-distributed Stochastic Neighbor Embedding) is a dimensionality reduction technique that tries to preserve local as well as global distribution. We looked at the distributions produced for each cancer type using TSNE and we notice two things: some outliers in cancer populations, that skew the scales, and distributions that don't seem to follow any obvious patterns in many cases.