In [48]:

```
import warnings
warnings.filterwarnings('always')

import pandas as pd
import urllib.request
import numpy as np
from IPython.display import display
from sklearn.model_selection import StratifiedKFold
from sklearn.naive_bayes import MultinomialNB
from sklearn.neighbors import KNeighborsClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import GridSearchCV
from sklearn import metrics
from sklearn import preprocessing
from sklearn.model_selection import train_test_split
import matplotlib.pyplot as plt
from sklearn.metrics import precision_recall_fscore_support
from sklearn.metrics import confusion_matrix
from textwrap import wrap
```

In [4]:

```
#TCGA dictionary information
tcga_dict = open("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 diction
ary
        dict_name_index += 1
    elif dict_name_index == 5:
        code_to_disease = eval(line)
```

In [5]:

```
def getDataAndLabels(cases):
    labels_string = cases.cancer_type
    le = preprocessing.LabelEncoder()
    labels = le.fit_transform(labels_string)

    # Get rid of the cancer type and patient_id columns
    data = cases[cases.columns[3:]]
    return {'data': data, 'labels': labels , 'label_encoder': le }
```

In [6]:

```
print('Loading case data ...')
cases_100 = pd.read_csv("pancancer_case_features_100.csv")
cases_250 = pd.read_csv("pancancer_case_features_250.csv")
cases_500 = pd.read_csv("pancancer_case_features_500.csv")
cases_800 = pd.read_csv("pancancer_case_features_800.csv")
all_data = {
    '100': getDataAndLabels(cases_100),
    '250': getDataAndLabels(cases_250),
    '500': getDataAndLabels(cases_500),
    '800': getDataAndLabels(cases_800)
}
print("done.")
```

```
Loading case data ...
done.
```

```
In [7]: def foldData(data, labels):
            skf = StratifiedKFold(n_splits=10)
            folds = []
            for train_index, dev_index in skf.split(data, labels):
                train_data, dev_data     = data.values[train_index], data.values[dev_index]
                train_labels, dev_labels = labels[train_index], labels[dev_index]
                folds.append( {'train_data': train_data, 'train_labels': train_labels,
                                'dev_data':   dev_data,   'dev_labels': dev_labels })
            return folds
```

```
In [21]: def splitData(data, labels):
             train_data_all, test_data, train_labels_all, test_labels = train_test_split(data, labe
         ls,
                                                                                             stratify=labels,
                                                                                             test_size=0.25)

             train_data, dev_data, train_labels, dev_labels = train_test_split(train_data_all, trai
         n_labels_all,
                                                                                                   stratify=train_labels
         _all,
                                                                                                   test_size=0.20)

             print("training data:", train_data.shape)
             print("dev data     :", dev_data.shape)
             print("test data    :",  test_data.shape)
             return {'train_data': train_data, 'train_labels': train_labels,
                     'dev_data':   dev_data,   'dev_labels': dev_labels,
                     'test_data':  test_data,  'test_labels': test_labels}
```

```
In [22]: def getBestParams(train_data, train_labels):
             mini_train_data, mini_test_data, mini_train_labels, mini_test_labels = train_test_spli
         t(train_data, train_labels,
                                                 stratify=train_labels,
                                                 test_size=0.55)

             #
             # Logistic Regression
             #
             lr = LogisticRegression(penalty='l2', multi_class = 'ovr', solver='liblinear', max_ite
         r=150)
             params = {'C': [0.001, 0.01, 0.1, 0.5, 1, 10]}
             logit = GridSearchCV(lr, params, cv=5,
                                  scoring='accuracy', return_train_score=True)

             # Fit  training data
             logit.fit(mini_train_data, mini_train_labels)
             # Show the best C parameter to use and the expected accuracy
             print('\nLogistic Regression Classifier, L2 regularization')
             print(' Best param:', logit.best_params_)
             print(' Accuracy:  ', np.round(logit.best_score_, 4) )

             return logit.best_params_
```

In [23]:

```
#
#  Find best C param for Logistic Regression L2
#
data   = all_data['100']['data']
labels = all_data['100']['labels']
splits = splitData(data, labels)
print("\nFinding best C for Logistic Regression, L2...\n")
logit_best_params = getBestParams(splits['train_data'], splits['train_labels'])
```

```
training data: (6004, 1063)
dev data     : (1502, 1063)
test data    : (2502, 1063)

Finding best C for Logistic Regression, L2...


/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_search.py:81
3: DeprecationWarning: The default of the `iid` parameter will change from True to False
in version 0.22 and will be removed in 0.24. This will change numeric results when test-s
et sizes are unequal.
  DeprecationWarning)

Logistic Regression Classifier, L2 regularization
 Best param: {'C': 0.5}
 Accuracy:    0.4532
```

In [24]:

```
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)
```

In [25]:

```
def plotMetrics(precision_l1, recall_l1, precision, recall,
                precision_by_label, recall_by_label,
                confusion, feature_size, label_encoder):
    labels = [ '\n'.join(wrap(l, 8)) for l in feature_size ]

    plt.rcParams["figure.figsize"] = (20,10)

    plt.plot(labels, precision, color='darkorange',
             linewidth=3, label='L2 precision with reduced number of features', marker='o'
)
    plt.plot(labels, recall, color='mediumblue', linestyle='dashed',
             linewidth=3, label='L2 recall with reduced number of features', marker='o' )

    plt.plot(labels, precision_l1, color='gray',alpha=.6,
             linewidth=3, label='L1 precision at different C values', marker='o' )
    plt.plot(labels, recall_l1, color='gray', linestyle='dashed',alpha=.6,
             linewidth=3, label='L1 at different C values', marker='o' )


    plt.yticks(np.arange(.34, .7, .01))
    plt.ylabel('Precision, Recall', fontsize=20)
    plt.xlabel('Feature size with L1 regularization at different C parameters', fontsize=2
0, labelpad=20)
    plt.legend()
    plt.grid()
    plt.show()

    # find optimal f1
    best_idx = np.argmax(precision)

    # Show precision and recall across different labels
    showPrecisionRecallPairByLabel(precision_by_label[best_idx], recall_by_label[best_idx
], label_encoder)


    # Get the confusion matrix for the optimal precision
    # Show the labels that have the highest error rate
    conf_mx = confusion[best_idx]
    showTopConfused(conf_mx, label_encoder)
```

In [26]:

```
def showTopConfused(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)

    max_coords = coords_of_max(norm_conf_mx, 10)
    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([ 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', 'error_rate', 'error
_count'])
    display(df)
```

```
In [44]: def showPrecisionRecallByLabel(precision_by_label, recall_by_label, label_encoder):
    labels = []
    for i in range(len(precision_by_label)):
        label = label_encoder.inverse_transform([i])[0]
        labels.append(label)

    y_pos = np.arange(len(labels))

    fig, ax = plt.subplots()

    width = .4

    ax.barh(y_pos,         precision_by_label, width, color="darkorange" , alpha=.7, label="precision")
    ax.barh(y_pos + width, recall_by_label,    width, color='mediumblue',  alpha=.7, label='recall')

    ax.set_yticks(y_pos)
    ax.set_yticklabels(labels)
    ax.invert_yaxis()  # labels read top-to-bottom

    ax.legend()

    ax.set_xlabel('Precision')
    ax.set_title('Cancer Type')
    plt.grid()
    plt.show()


def showPrecisionRecallPairByLabel(precision_by_label, recall_by_label, label_encoder):
    labels = []
    for i in range(len(precision_by_label)):
        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.yaxis.tick_right()

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

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

    ax1.barh(y_pos, precision_by_label, color="darkorange" , alpha=.7, label="precision")
    ax2.barh(y_pos, recall_by_label,    color='mediumblue',  alpha=.7, label='recall')

    ax1.set_title('Precision')
    ax2.set_title('Recall')

    plt.grid()
    plt.show()
```

In [45]:

```
def runLogitL1(train_data, train_labels, dev_data, dev_labels, c_param):
    l1 = LogisticRegression(penalty='l1', tol=.01,
                            solver="liblinear", multi_class="ovr",
                            max_iter=500, C=c_param)
    # Fit model
    l1.fit(train_data, train_labels)
    # Predict
    predict = l1.predict(dev_data)
    # Get precision, recall, f1 scores
    scores = precision_recall_fscore_support(dev_labels, predict, average='weighted', labe
ls=np.unique(predict))

    # Get the features with non-zero coefficients.  We will use
    # this list to reduce the features for the
    # following logistic regression with L2 regularization
    non_zero_sums = np.where(np.sum(l1.coef_, axis=0) != 0)
    names = np.array(list(train_data.columns))
    non_zero_names = names[non_zero_sums]

    return {'scores': scores, 'non_zero_genes': non_zero_names}
```

```
In [46]: def eliminateFeatures(train_data, train_labels, dev_data, dev_labels, logit_best_params, l
         abel_encoder):

             params = {'C':  [1000, 100, 10, 1, .5, .3, .1, .05]}


             # Now perform logistic regression on this training set with reduced features
             # as well as the orginal non-reduced training set.  Run over different
             # C values to plot differences in accuracy
             precision_l1        = []
             recall_l1           = []

             precision           = []
             recall              = []
             precision_by_label  = []
             recall_by_label     = []
             feature_size        = []
             confusion           = []


             for c_param in reversed(params['C']):
                 # Keep this random seed here to make comparison easier.
                 np.random.seed(0)

                 #
                 # Perform Logistic Regression on different C values
                 # using L1 regularization
                 #
                 l1_info = runLogitL1(train_data, train_labels, dev_data, dev_labels, c_param)
                 non_zero_genes = l1_info['non_zero_genes']
                 feature_size.append(str(len(non_zero_genes)) + ' (C=' + str(c_param) + ")")
                 precision_l1.append(l1_info['scores'][0])
                 recall_l1.append(l1_info['scores'][1])


                 #
                 # Reduce feature size, only keeping features with non-zero weights
                 # found using l1 regularization
                 #
                 min_train_data = train_data[non_zero_genes]
                 min_dev_data   = dev_data[non_zero_genes]


                 # Run logistic regression with L2 regularization on reduced
                 # feature set
                 lr = LogisticRegression(penalty='l2', tol=.01, max_iter=150,
                                         C=logit_best_params['C'], solver="liblinear", multi_class=
         "ovr")
                 lr.fit(min_train_data, train_labels)

                 predict = lr.predict(min_dev_data)

                 # Get precision, recall, f1 scores
                 scores = precision_recall_fscore_support(dev_labels, predict, average='weighted',
         labels=np.unique(predict))
                 scores_by_label = precision_recall_fscore_support(dev_labels, predict, average=Non
         e)

                 # Get confusion matrix
                 confusion_mx = confusion_matrix(dev_labels, predict)

                 precision.append(scores[0])
                 recall.append(scores[1])
                 precision_by_label.append(scores_by_label[0])
```

```
        recall_by_label.append(scores_by_label[1])
        confusion.append(confusion_mx)

    plotMetrics(precision_l1, recall_l1, precision, recall,
                precision_by_label, recall_by_label,
                confusion, feature_size, label_encoder)
```

In [49]:

```
#
#  Run classifier on each binary matrix, that has different
#  number of columns (genes).  Iterate through different
#  C values, using Logistic Regression L1 regularization
#  to eliminate features.  Now run Logistic Regression, L2
#  regularization and keep track of precision, recall,
#  and confusion matrix.  Plot these metrics per feature
#  size and show the confusion matrix for the best performing
#  feature size.
#
for top_n_genes, data_object in all_data.items():
    data          = data_object['data']
    labels        = data_object['labels']
    label_encoder = data_object['label_encoder']
    splits = splitData(data, labels)
    eliminateFeatures(splits['train_data'], splits['train_labels'],
                      splits['dev_data'], splits['dev_labels'], logit_best_params, label_e
ncoder)
```

```
training data: (6004, 1063)
dev data     : (1502, 1063)
test data    : (2502, 1063)
```

```
/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
7: UndefinedMetricWarning: Precision and F-score are ill-defined and being set to 0.0 in
labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
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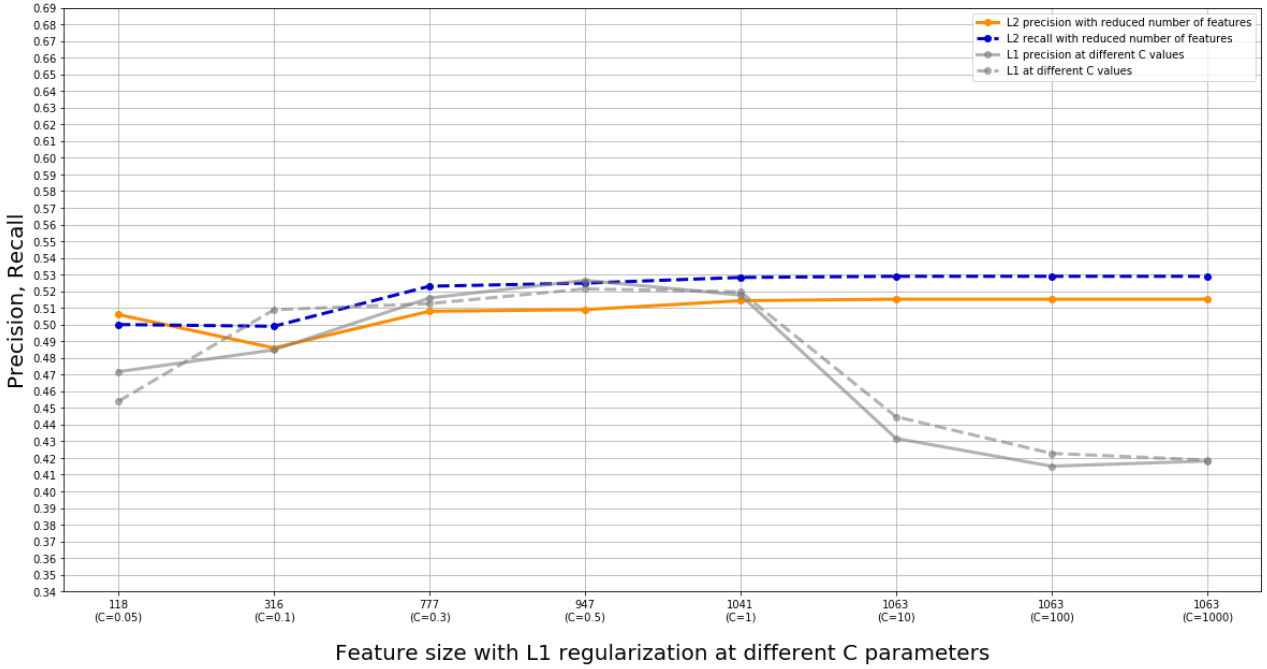
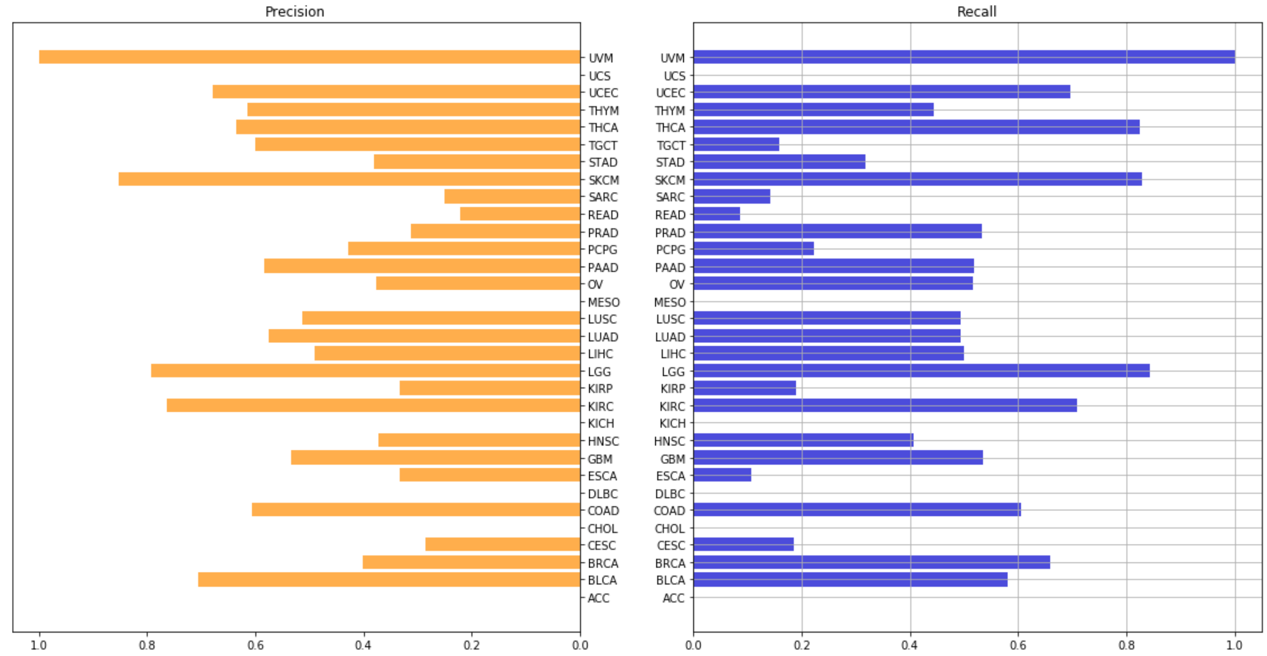
```





	actual	predicted	error_rate	error_count
0	Cholangiocarcinoma	Kidney_renal_clear_cell_carcinoma	0.400000	2
1	Kidney_Chromophobe	Prostate_adenocarcinoma	0.400000	4
2	Adrenocortical_carcinoma	Breast_invasive_carcinoma	0.357143	5
3	Rectum_adenocarcinoma	Colon_adenocarcinoma	0.347826	8
4	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Cervical_squamous_cell_carcinoma_and_endocervi...	0.333333	2
5	Uterine_Carcinosarcoma	Uterine_Corpus_Endometrial_Carcinoma	0.333333	3
6	Mesothelioma	Breast_invasive_carcinoma	0.333333	4
7	Pheochromocytoma_and_Paraganglioma	Prostate_adenocarcinoma	0.296296	8
8	Testicular_Germ_Cell_Tumors	Prostate_adenocarcinoma	0.263158	5
9	Pheochromocytoma_and_Paraganglioma	Thyroid_carcinoma	0.259259	7

```
training data: (6004, 2530)
dev data     : (1502, 2530)
test data    : (2502, 2530)
```

```
/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
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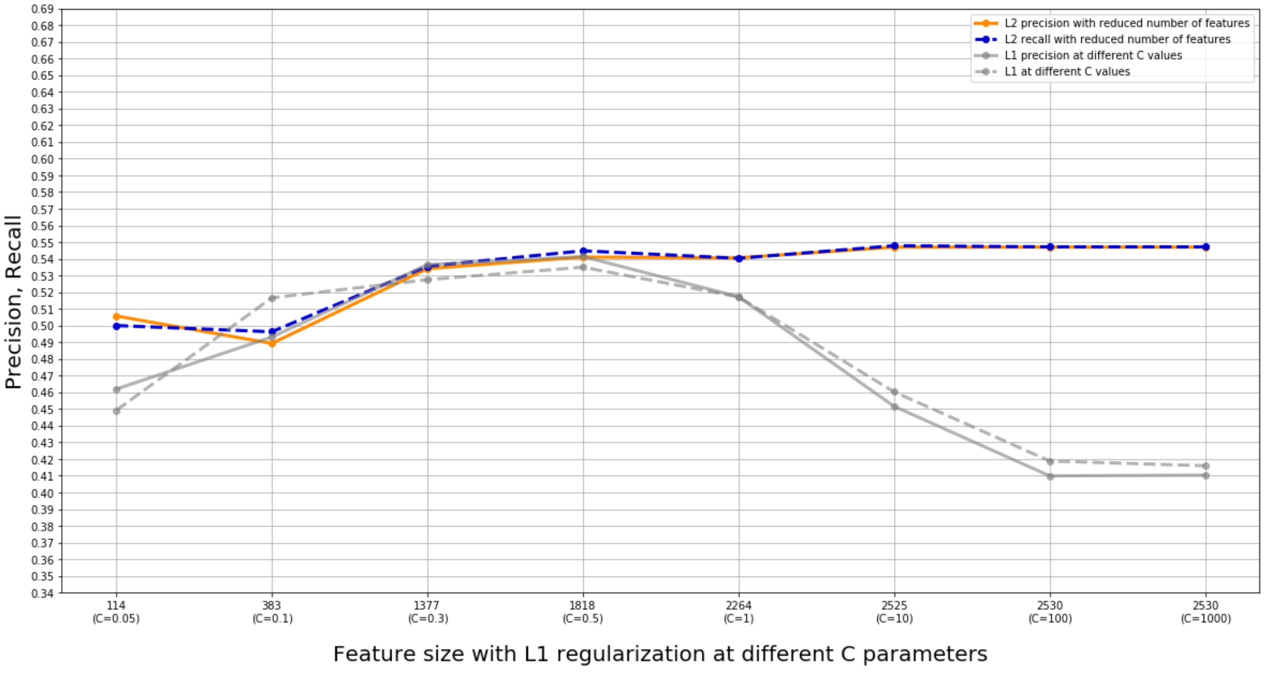

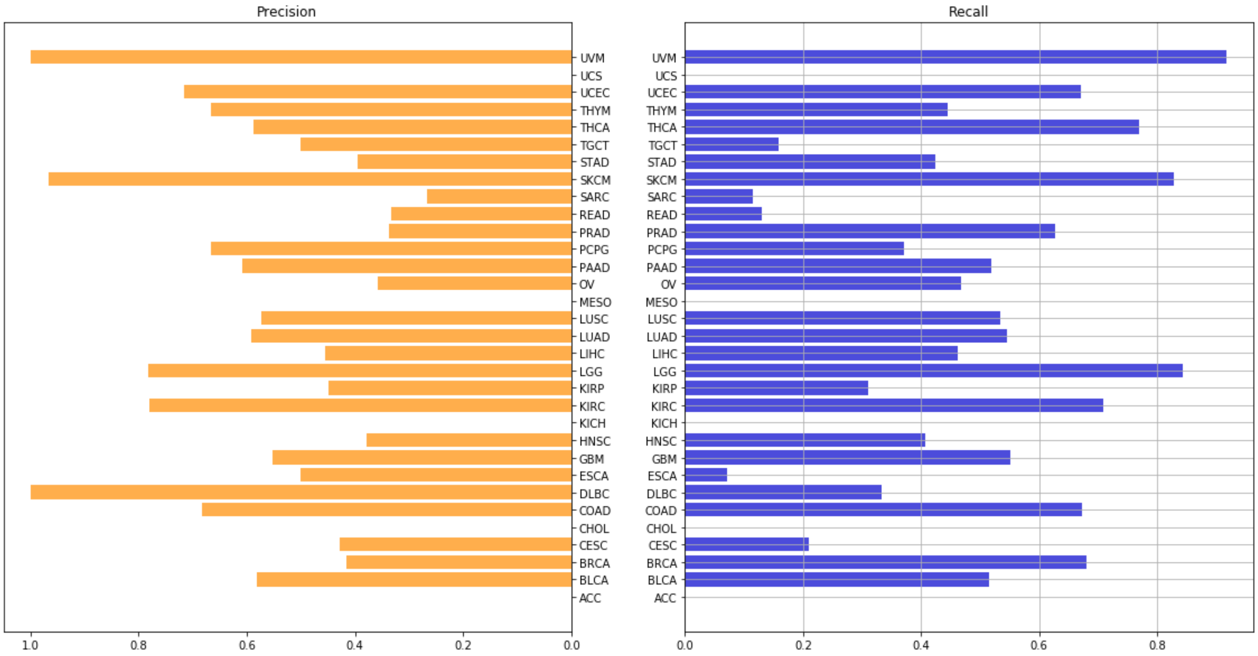

	actual	predicted	error_rate	error_count
0	Adrenocortical_carcinoma	Breast_invasive_carcinoma	0.428571	6
1	Mesothelioma	Prostate_adenocarcinoma	0.416667	5
2	Cholangiocarcinoma	Kidney_renal_clear_cell_carcinoma	0.400000	2
3	Rectum_adenocarcinoma	Colon_adenocarcinoma	0.347826	8
4	Uterine_Carcinosarcoma	Uterine_Corpus_Endometrial_Carcinoma	0.333333	3
5	Pheochromocytoma_and_Paraganglioma	Thyroid_carcinoma	0.333333	9
6	Mesothelioma	Breast_invasive_carcinoma	0.333333	4
7	Kidney_Chromophobe	Thyroid_carcinoma	0.300000	3
8	Kidney_Chromophobe	Prostate_adenocarcinoma	0.300000	3
9	Sarcoma	Breast_invasive_carcinoma	0.285714	10

```
training data: (6004, 4778)
dev data     : (1502, 4778)
test data    : (2502, 4778)
```

```
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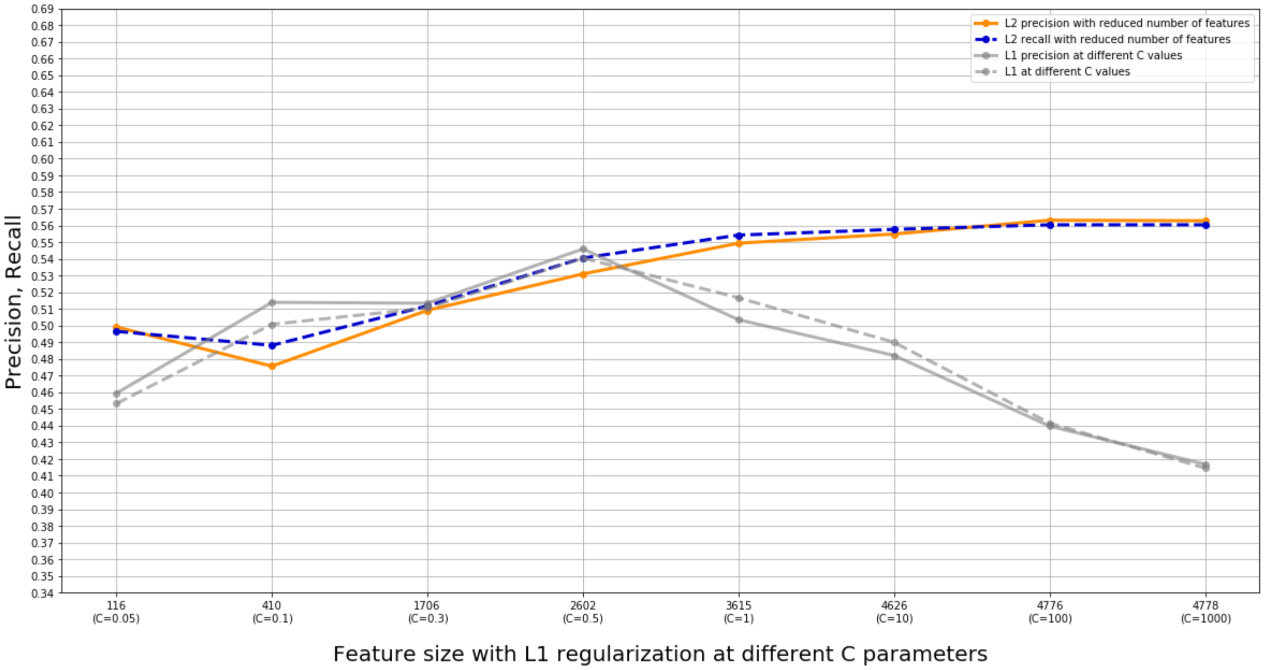
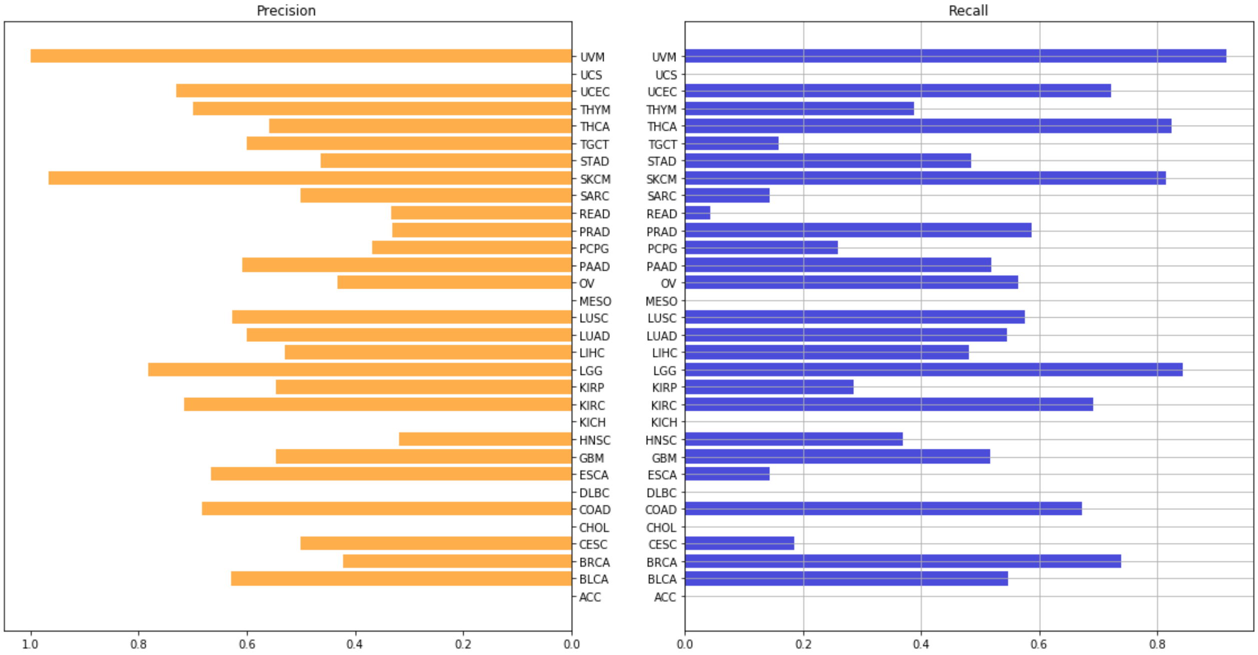
  'precision', 'predicted', average, warn_for)
```





	actual	predicted	error_rate	error_count
0	Kidney_Chromophobe	Thyroid_carcinoma	0.400000	4
1	Cholangiocarcinoma	Kidney_renal_clear_cell_carcinoma	0.400000	2
2	Rectum_adenocarcinoma	Colon_adenocarcinoma	0.391304	9
3	Thymoma	Prostate_adenocarcinoma	0.388889	7
4	Uterine_Carcinosarcoma	Uterine_Corpus_Endometrial_Carcinoma	0.333333	3
5	Mesothelioma	Prostate_adenocarcinoma	0.333333	4
6	Pheochromocytoma_and_Paraganglioma	Prostate_adenocarcinoma	0.333333	9
7	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Breast_invasive_carcinoma	0.333333	2
8	Mesothelioma	Breast_invasive_carcinoma	0.333333	4
9	Testicular_Germ_Cell_Tumors	Breast_invasive_carcinoma	0.315789	6

```
training data: (6004, 7184)
dev data     : (1502, 7184)
test data    : (2502, 7184)
```

```
/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
7: UndefinedMetricWarning: Precision and F-score are ill-defined and being set to 0.0 in
labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
7: UndefinedMetricWarning: Precision and F-score are ill-defined and being set to 0.0 in
labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
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/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
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/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
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/Users/tonyd/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.py:143
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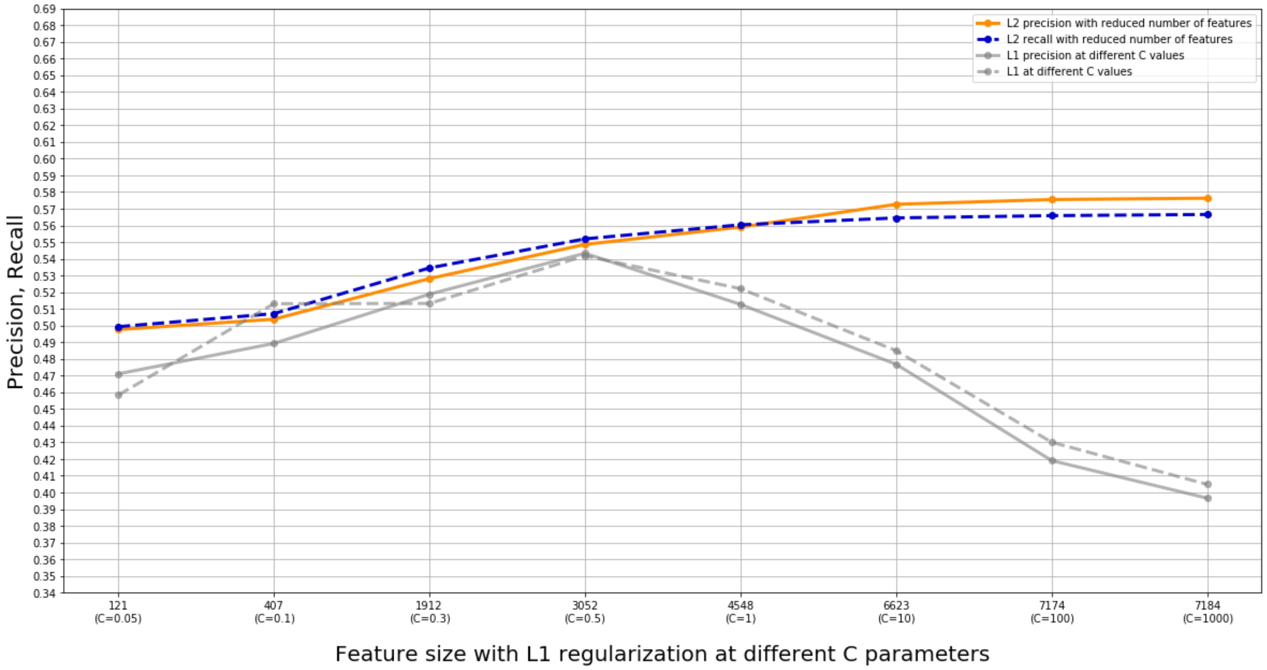
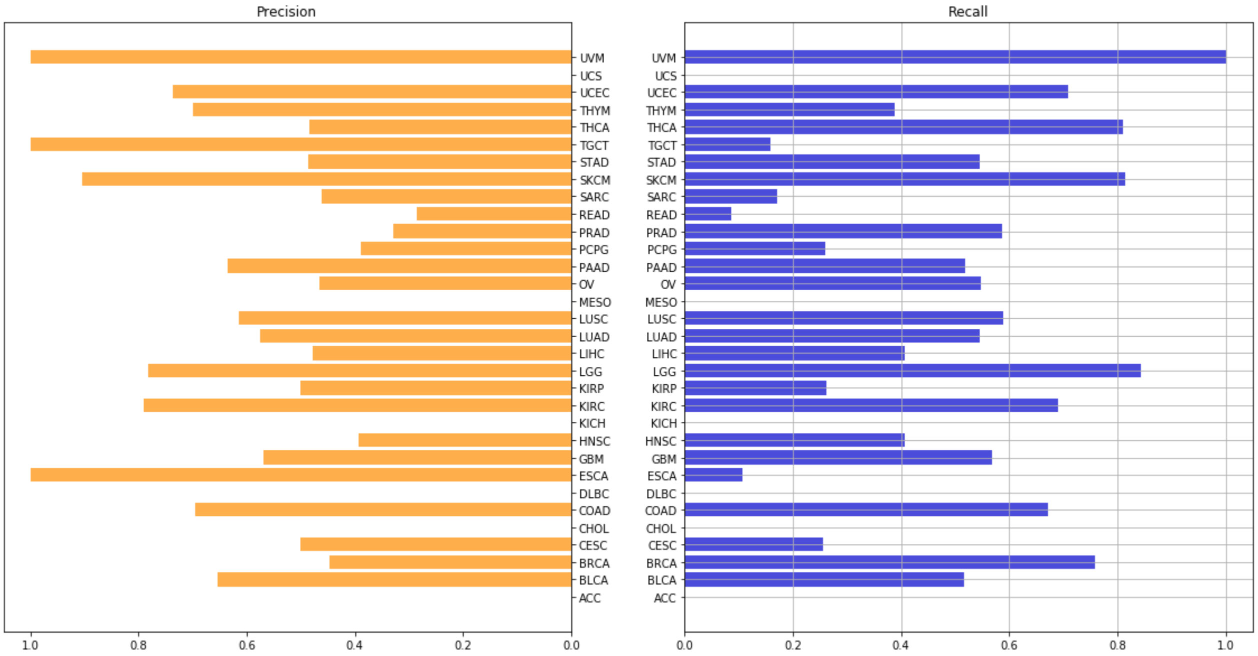
labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
```





	actual	predicted	error_rate	error_count
0	Pheochromocytoma_and_Paraganglioma	Thyroid_carcinoma	0.481481	13
1	Mesothelioma	Prostate_adenocarcinoma	0.416667	5
2	Cholangiocarcinoma	Kidney_renal_clear_cell_carcinoma	0.400000	2
3	Kidney_Chromophobe	Thyroid_carcinoma	0.400000	4
4	Rectum_adenocarcinoma	Colon_adenocarcinoma	0.391304	9
5	Adrenocortical_carcinoma	Thyroid_carcinoma	0.357143	5
6	Lymphoid_Neoplasm_Diffuse_Large_B-cell_Lymphoma	Liver_hepatocellular_carcinoma	0.333333	2
7	Uterine_Carcinosarcoma	Uterine_Corpus_Endometrial_Carcinoma	0.333333	3
8	Uterine_Carcinosarcoma	Breast_invasive_carcinoma	0.333333	3
9	Thymoma	Prostate_adenocarcinoma	0.333333	6

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In [ ]:
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In [ ]:
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