Capstone project - breast cancer

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Data set description

Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image. n the 3-dimensional space is that described in: [K. P. Bennett and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets", Optimization Methods and Software 1, 1992, 23-34].

Attribute information:

Ten real-valued features are computed for each cell nucleus: a) radius (mean of distances from center to points on the perimeter) b) texture (standard deviation of gray- scale values) c) perimeter d) area e) smoothness (local variation in radius lengths) f) compactness (perimeter^2 / area - 1.0) g) concavity (severity of concave portions of the contour) h) concave points (# of concave portions of the contour) i) symmetry j) fractal dimension ("coastline approximation" - 1)

The mean, standard error and "worst" or largest (mean of the three largest values) of these features were computed for each image, resulting in 30 features. For instance, field 3 is Mean Radius, field 13 is Radius SE, field 23 is Worst Radius.

Class distribution: 357 benign, 212 malignant

Data processing

1. Load and inspect data

In [135]:
```
## Load packages
import numpy as np # linear algebra
import pandas as pd # data processing, CSV file I/O (e.g. pd.read_csv)
import seaborn as sns # data visualization library
import matplotlib.pyplot as plt
# Input data files are available in the "../input/" directory.
# For example, running this (by clicking run or pressing Shift+Enter)
will list the files in the input directory
import time
from subprocess import check_output
print(check_output(["ls", "../input"]).decode("utf8"))
```

```
data.csv
```

In [136]:
```
data = pd.read_csv('../input/data.csv')
data.head()
```

Out[136]:

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smo
0	842302	M	17.99	10.38	122.80	1001.0	0.11
1	842517	M	20.57	17.77	132.90	1326.0	0.08
2	84300903	M	19.69	21.25	130.00	1203.0	0.10
3	84348301	M	11.42	20.38	77.58	386.1	0.14
4	84358402	M	20.29	14.34	135.10	1297.0	0.10

5 rows × 33 columns

The key findings are column 32 is all NAs, which will not be included in further analysis. Column diagnosis is the target column, contain the diagnosis results - M or B.

In [137]:
```
## column 32 is all NAN, can be deleted during analysis
data.iloc[:,32].unique()

data.iloc[:,1].unique()
```

Out[137]:
```
array(['M', 'B'], dtype=object)
```

2. Assess missing values

There is no missing values in the data set.

In [138]:
```
print(data.isnull().sum())
```

```
id                          0
diagnosis                   0
radius_mean                 0
texture_mean                0
perimeter_mean              0
area_mean                   0
smoothness_mean             0
compactness_mean            0
concavity_mean              0
concave points_mean         0
symmetry_mean               0
fractal_dimension_mean      0
radius_se                   0
texture_se                  0
perimeter_se                0
area_se                     0
smoothness_se               0
compactness_se              0
concavity_se                0
concave points_se           0
symmetry_se                 0
fractal_dimension_se        0
radius_worst                0
texture_worst               0
perimeter_worst             0
area_worst                  0
smoothness_worst            0
compactness_worst           0
concavity_worst             0
concave points_worst        0
symmetry_worst              0
fractal_dimension_worst     0
Unnamed: 32               569
dtype: int64
```

3. Standardize data

In [139]:
```
## transform data for plotting
data_trans = data.drop(['id','diagnosis','Unnamed: 32'], axis=1)
data_trans = (data_trans - data_trans.mean()) / data_trans.std() ## st
andardization
data_trans['diagnosis'] = data.diagnosis
data_trans_melt = pd.melt(data_trans, id_vars = "diagnosis", var_name
= "features", value_name = "value")
```

In [140]:
```
data_trans_melt.tail()
```

Out[140]:

	diagnosis	features	value
17065	M	fractal_dimension_worst	-0.708467
17066	M	fractal_dimension_worst	-0.973122
17067	M	fractal_dimension_worst	-0.318129
17068	M	fractal_dimension_worst	2.217684
17069	B	fractal_dimension_worst	-0.750546

Exploratory analysis

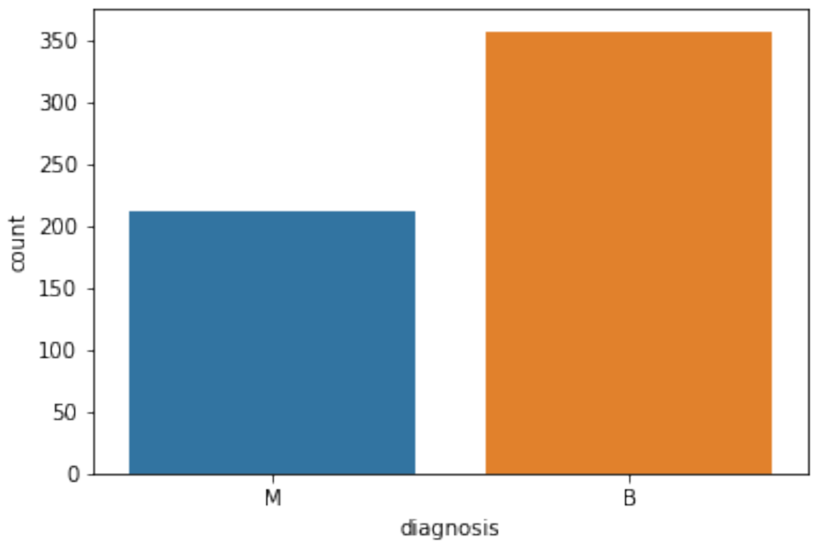
1. Visualize data

Count is plot is to inspect the distribution of malignant vs benign.

In [141]:
```
## make diagnosis result in one list, features in one list
x = data.drop(['id', 'diagnosis', 'Unnamed: 32'], axis=1)
y = data.diagnosis
```

In [142]:
```
## Plot the count of each diagnosis
ax = sns.countplot(y, label='Count')
B, M = y.value_counts()
print('Number of Benign: ',B)
print('Number of Malignant: ', M)
```

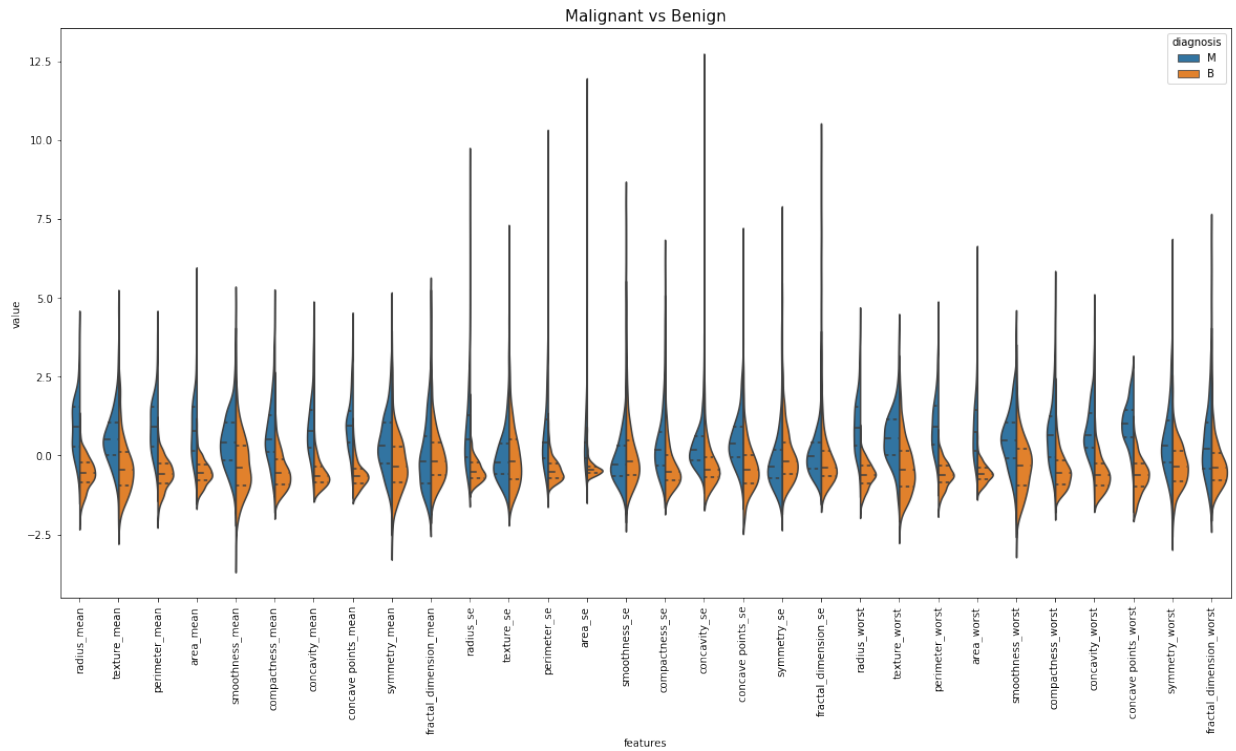
```
Number of Benign:  357
Number of Malignant:  212
```



Violin plot is used to exam the ditribution of each features. Features differ a lot between malignant and benign will be considered to include the the model.

In [143]:
```
plt.figure(figsize = (20,10))
sns.violinplot(x="features", y="value", hue="diagnosis", data=data_trans_melt, split=True, inner="quart")
plt.xticks(rotation=90)
plt.title("Malignant vs Benign", fontdict={"fontsize":15})
```

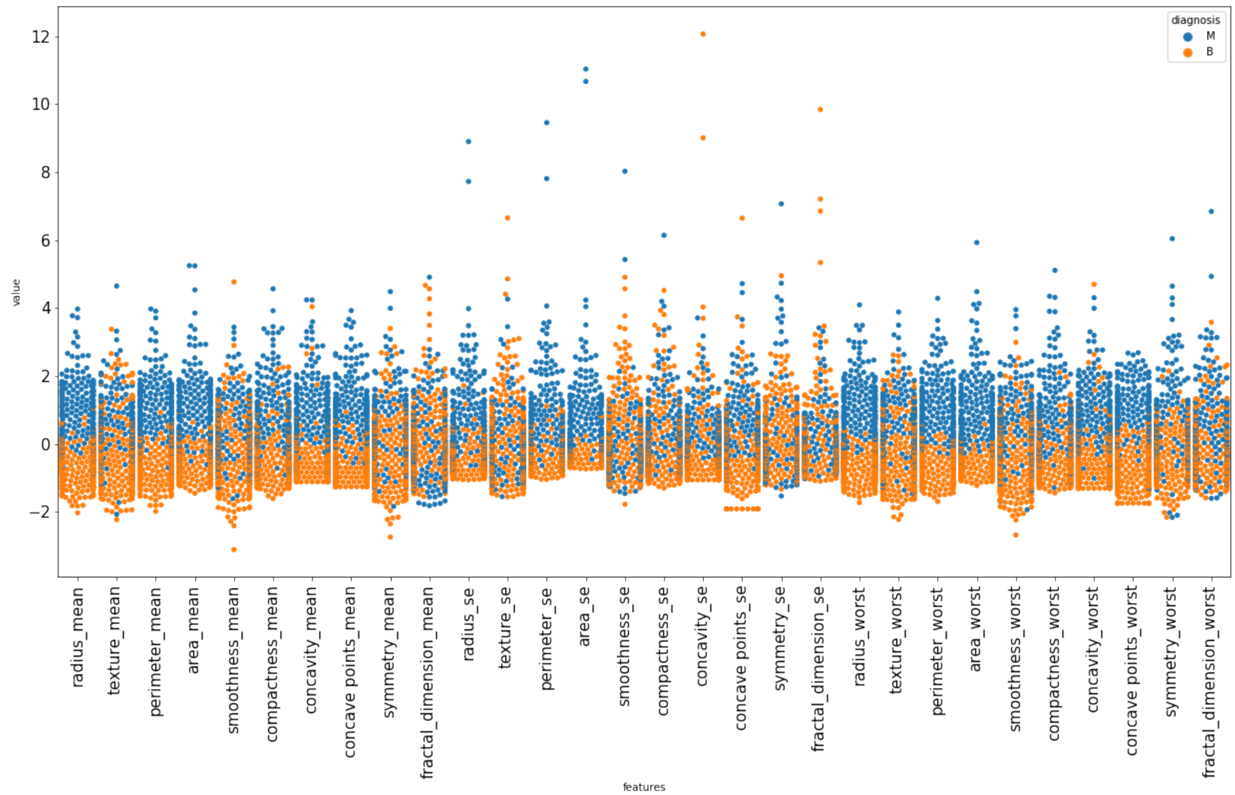
Out[143]: Text(0.5,1,'Malignant vs Benign')



- Based on the violin plot, benign samples in general have lower values than malignant
- There are lots of outliers of each feature
- Features with significant difference: radias_mean, concavity_mean, concave points points_mean, area_se, lots of features in "worst"

Swarm plot is used to better visualize the data

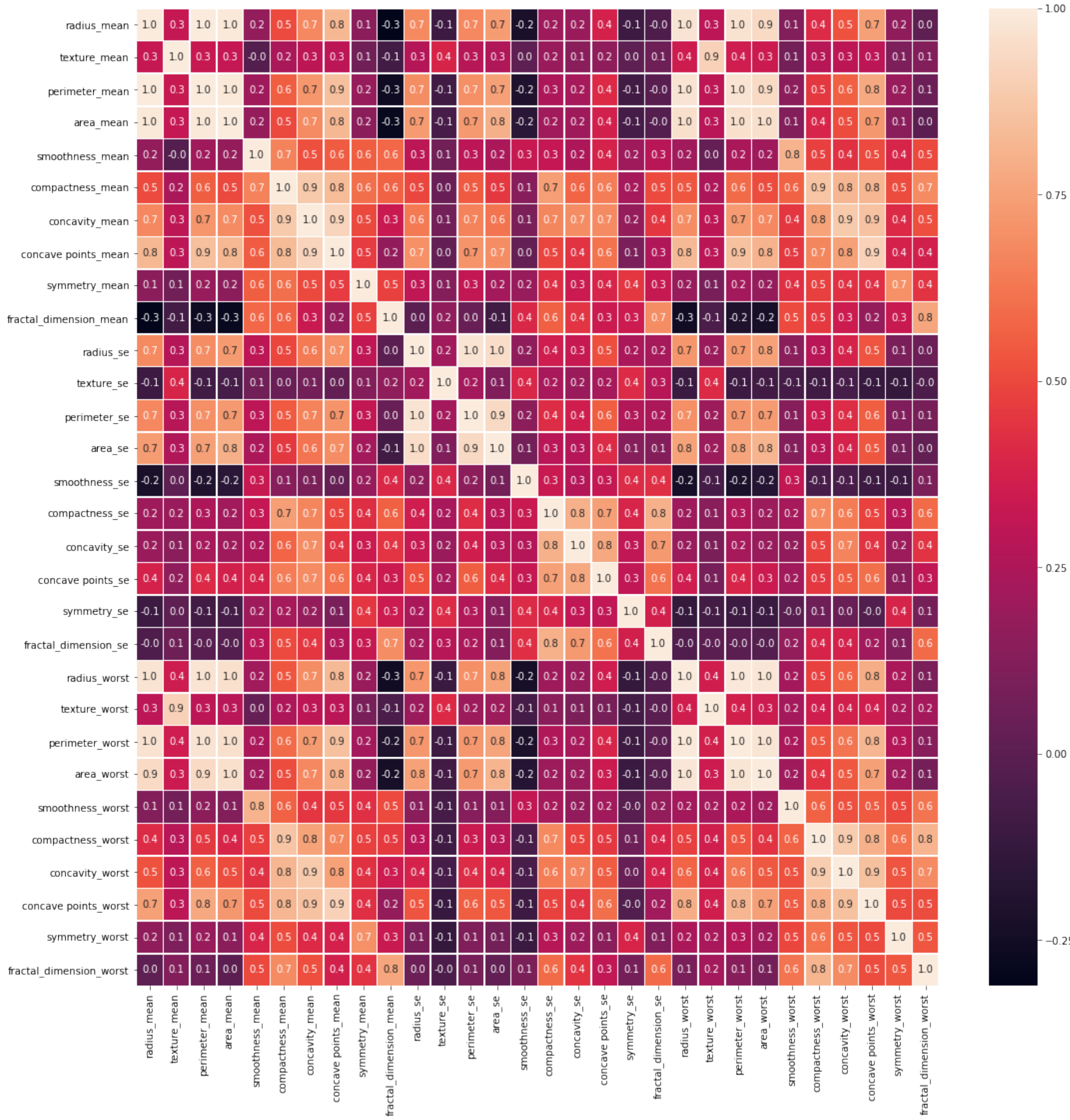
In [49]:
```
plt.figure(figsize = (20,10))
ax = sns.swarmplot(x="features", y="value", hue= "diagnosis", data=dat
a_trans_melt)
plt.xticks(rotation = 90)
ax.tick_params(labelsize = 15)
```



2. Evaluate multi-collinearity through heat map

In [13]:
```
f,ax = plt.subplots(figsize=(18, 18))
sns.heatmap(x.corr(), annot=True, linewidths=.5, fmt= '.1f',ax=ax)
```

Out[13]: <matplotlib.axes._subplots.AxesSubplot at 0x1a30f22d30>



From the heat map, we can see there are lots of features corelated with each other - multicollinearity . This indicates that we should do feature selection and PCA to address this issue.

__3. PCA to addresss multicollinearity and get benchmark for predictive model performance

In [144]:
```
x_trans = data_trans.drop(['diagnosis'], axis=1)
x_trans.head()
```

Out[144]:

	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	comp
0	1.096100	-2.071512	1.268817	0.983510	1.567087	3.280
1	1.828212	-0.353322	1.684473	1.907030	-0.826235	-0.48
2	1.578499	0.455786	1.565126	1.557513	0.941382	1.052
3	-0.768233	0.253509	-0.592166	-0.763792	3.280667	3.399
4	1.748758	-1.150804	1.775011	1.824624	0.280125	0.538

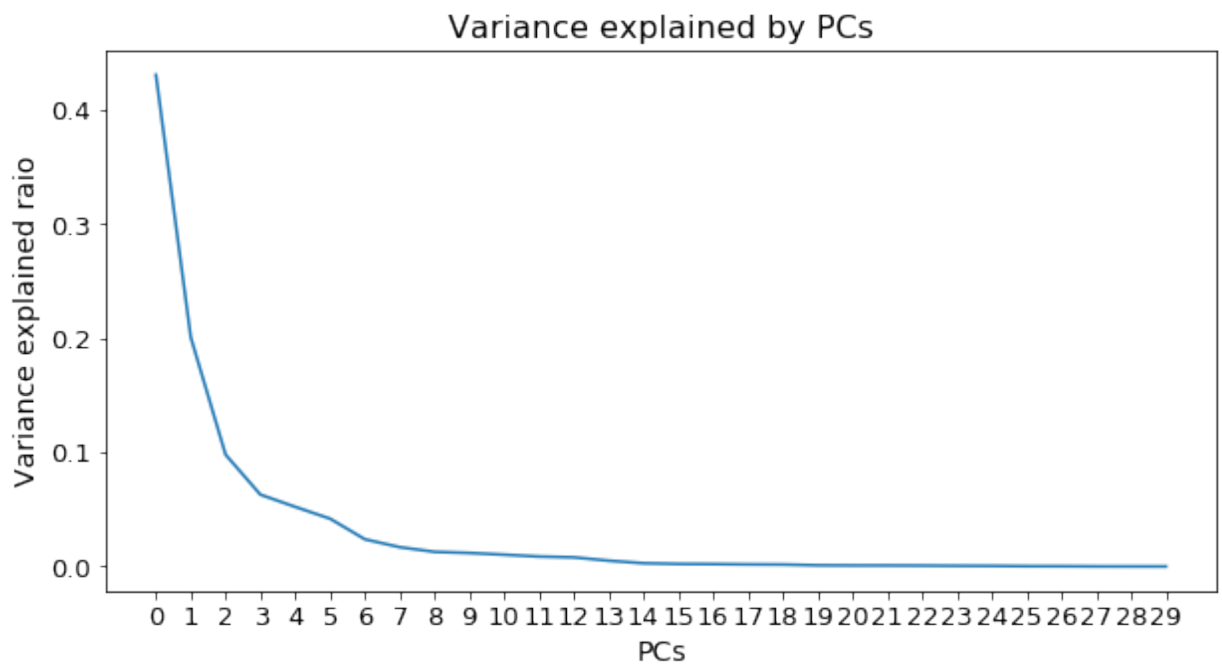
5 rows × 30 columns

In [145]:
```
## split the dataset into training and testing
from sklearn.model_selection import train_test_split


# split data train 70 % and test 30 %
x_train, x_test, y_train, y_test = train_test_split(x_trans, y, test_s
ize=0.3, random_state=42)

## PCA on training data and plot the percentage of variance explained
from sklearn.decomposition import PCA
pca = PCA()
pca.fit_transform(x_train)
plt.figure(figsize = (10,5))
pcs = np.arange(pca.n_components_)
plt.plot(pcs, pca.explained_variance_ratio_)
plt.xticks(pcs, fontsize = 13)
plt.yticks(fontsize = 13)
plt.xlabel("PCs", fontsize = 14)
plt.ylabel("Variance explained raio", fontsize = 14)
plt.title("Variance explained by PCs", fontsize = 16)
```

```
Out[145]: Text(0.5,1,'Variance explained by PCs')
```



The first **six** capture the most variance in data set. We next look at what original features contribute to the first six PCs and they can considered include in the model.

```
In [146]: variance_from_feature = pd.DataFrame(pca.components_, columns = list(d
ata)[2:32])
variance_from_feature.T.iloc[:,:6]  ## look at the first six PCs
```

Out[146]:

	0	1	2	3	4	
radius_mean	0.222656	-0.229404	-0.020918	-0.035382	0.061762	0.02335
texture_mean	0.105219	-0.039244	0.036707	0.611434	-0.048591	-0.0806
perimeter_mean	0.230670	-0.210681	-0.021514	-0.037227	0.061470	0.01893
area_mean	0.229600	-0.229335	0.017267	-0.054361	0.024496	-0.0026
smoothness_mean	0.136608	0.181331	-0.124076	-0.157794	-0.384644	-0.2232
compactness_mean	0.229308	0.162642	-0.078284	-0.041616	0.020095	-0.0254
concavity_mean	0.254258	0.068014	-0.005365	-0.030366	0.096398	-0.0330
concave points_mean	0.257850	-0.026583	-0.047610	-0.062613	-0.033636	-0.0388
symmetry_mean	0.142883	0.180462	-0.057396	-0.026522	-0.231231	0.37600
fractal_dimension_mean	0.054644	0.372087	-0.016567	-0.085780	-0.071313	-0.1243

radius_se	0.222084	-0.114349	0.269018	-0.089685	-0.193415	-0.0112
texture_se	0.035205	0.093577	0.316194	0.363017	-0.199626	0.01534
perimeter_se	0.225763	-0.093140	0.272784	-0.077251	-0.147647	0.00931
area_se	0.221917	-0.161825	0.228757	-0.114406	-0.176612	-0.0460
smoothness_se	0.026898	0.207082	0.310815	-0.042212	-0.276929	-0.2903
compactness_se	0.164496	0.241724	0.161598	0.046235	0.269361	0.06151
concavity_se	0.153924	0.202542	0.200424	0.007370	0.351097	0.00728
concave points_se	0.185208	0.146886	0.227056	-0.029102	0.195635	-0.0137
symmetry_se	0.052624	0.152600	0.241498	-0.010957	-0.232154	0.53910
fractal_dimension_se	0.100984	0.287197	0.221423	-0.031191	0.242697	-0.0454
radius_worst	0.229312	-0.212533	-0.064959	-0.011524	0.018217	-0.0014
texture_worst	0.104381	-0.027828	-0.077596	0.635573	-0.083098	-0.0837
perimeter_worst	0.236585	-0.190606	-0.064909	-0.008323	0.033143	0.00274
area_worst	0.229665	-0.213263	-0.028610	-0.028797	-0.011999	-0.0348
smoothness_worst	0.122394	0.177181	-0.283641	-0.044351	-0.346219	-0.3251
compactness_worst	0.191616	0.151784	-0.226346	0.069940	0.127467	0.02539
concavity_worst	0.216423	0.101187	-0.169218	0.042960	0.188203	-0.0146
concave points_worst	0.244612	0.007480	-0.188201	-0.000303	0.052081	-0.0242
symmetry_worst	0.119425	0.126063	-0.302632	0.048945	-0.174072	0.52603
fractal_dimension_worst	0.115315	0.280038	-0.215836	0.011908	0.072457	-0.0833

The top 2 variables of the first six PCs are summarized below. They can be considered to include in the model.
PC1: concavity_mean, concavity points_mean
PC2: fractal_dimension_mean, fractal_dimension_wrost
PC3: texture_se, smootheness_se
PC4: texture_mean, texture_wrost
PC5: smoothness_mean, concavity_se
PC6: symmetry_se, symmetry_wrost

4. Hand selected features

Based on the matrix correlation and PCA, I handed selected the following 6 features: concavity_mean, fractal_dimension_mean, fractal_dimension_wrost, texture_se, smootheness_se, texture_wrost

Classification Models

Model I: Logistic regression

From data exploratory analysis, we know that multi-linearality exists. We exame the performance of using **all data, hand-selected features and sklearn selected feature** with logistic regession.

Logistic regression on all features

In [147]:
```
## functions to compute the model performance matrix
# Import metrics functions from sklearn
from sklearn.metrics import precision_score, accuracy_score, recall_sc
ore, f1_score, roc_auc_score
# Helper method to print metric scores
def get_performance_metrics(y_train, p_train_pred, y_test, p_test_pred
, threshold=0.5):
    metric_names = ['AUC','Accuracy','Precision','Recall','f1-score']
    metric_values_train = [roc_auc_score(y_train, p_train_pred),
                    accuracy_score(y_train, p_train_pred>threshold),
                    precision_score(y_train, p_train_pred>threshold),
                    recall_score(y_train, p_train_pred>threshold),
                    f1_score(y_train, p_train_pred>threshold)
                   ]
    metric_values_test = [roc_auc_score(y_test, p_test_pred),
                    accuracy_score(y_test, p_test_pred>threshold),
                    precision_score(y_test, p_test_pred>threshold),
                    recall_score(y_test, p_test_pred>threshold),
                    f1_score(y_test, p_test_pred>threshold)
                   ]
    all_metrics = pd.DataFrame({'metrics':metric_names,
                                'train':metric_values_train,
                                'test':metric_values_test},columns=['m
etrics','train','test']).set_index('metrics')
    print(all_metrics)
```

In [148]:
```
## convert the y into binary model
y_train_binary = y_train
y_test_binary = y_test
y_train_binary = y_train_binary.replace(['M'], 1)
y_test_binary = y_test_binary.replace(['M'], 1)
y_train_binary = y_train_binary.replace(['B'], 0)
y_test_binary = y_test_binary.replace(['B'], 0)
```

In [149]:
```
np.shape(x_train)
```

Out[149]:
```
(398, 30)
```

In [150]:
```
# Import logistic regression from sklearn
from sklearn.linear_model import LogisticRegression

# Initialize model by providing parameters
# http://scikit-learn.org/stable/modules/generated/sklearn.linear_mode
l.LogisticRegression.html
#clf = LogisticRegression(C=1.0, penalty='l2')
clf = LogisticRegression()
# Fit a model by providing X and y from training set
clf.fit(x_train, y_train_binary)

# Make prediction on the training data
y_train_pred = clf.predict(x_train)
p_train_pred = clf.predict_proba(x_train)[:,1]

# Make predictions on test data
y_test_pred = clf.predict(x_test)
p_test_pred = clf.predict_proba(x_test)[:,1]
```

1. Logistic regression with full data set

In [151]:
```
# print model results
get_performance_metrics(y_train_binary, p_train_pred, y_test_binary, p
_test_pred)
```

```
              train      test
metrics
AUC        0.997143  0.998089
Accuracy   0.987437  0.982456
Precision  0.993151  0.968750
Recall     0.973154  0.984127
f1-score   0.983051  0.976378
```

2. Logistic regression with 6 hand-selected features

In [152]:
```
#selected_features = [u'texture_se', u'smoothness_se', u'texture_worst
']
selected_features = [u'concavity_mean', u'fractal_dimension_mean', u'f
ractal_dimension_worst', u'texture_se', u'smoothness_se', u'texture_wo
rst']
x_train_handSelected = x_train[selected_features]
x_test_handSelected = x_test[selected_features]
#clf = LogisticRegression(C=1.0, penalty='l2')
clf = LogisticRegression()
# Fit a model by providing X and y from training set
clf.fit(x_train_handSelected, y_train_binary)

# Make prediction on the training data
y_train_pred = clf.predict(x_train_handSelected)
p_train_pred = clf.predict_proba(x_train_handSelected)[:,1]

# Make predictions on test data
y_test_pred = clf.predict(x_test_handSelected)
p_test_pred = clf.predict_proba(x_test_handSelected)[:,1]
get_performance_metrics(y_train_binary, p_train_pred, y_test_binary, p
_test_pred)
```

```
              train      test
metrics
AUC        0.974367  0.981922
Accuracy   0.932161  0.953216
Precision  0.917808  0.936508
Recall     0.899329  0.936508
f1-score   0.908475  0.936508
```

Out[152]: 0.9532163742690059

3. Logistic regression with cross validation & grid search with all features

In [ ]:
```
# define function to perform train, test, and get model performance
def train_test_model(clf, X_train, y_train, X_test, y_test):
    # Fit a model by providing X and y from training set
    clf.fit(X_train, y_train)

    # Make prediction on the training data
    y_train_pred = clf.predict(X_train)
    p_train_pred = clf.predict_proba(X_train)[:,1]

    # Make predictions on test data
    y_test_pred = clf.predict(X_test)
    p_test_pred = clf.predict_proba(X_test)[:,1]

    # print model results
    get_performance_metrics(y_train, p_train_pred, y_test, p_test_pred
)
    #plot_roc_curve(y_train, p_train_pred, y_test, p_test_pred)
```

In [162]:
```
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import make_scorer, roc_auc_score, accuracy_score
from sklearn.model_selection import GridSearchCV

# Choose the type of classifier.
clf = LogisticRegression()

# Choose some parameter combinations to try
param_grid = {'C': [0.5,1.5],
              'max_iter': [50,150]
             }

# Type of scoring used to compare parameter combinations
acc_scorer = make_scorer(roc_auc_score)

# Run the grid search
# read theory
grid_obj = GridSearchCV(clf, param_grid, cv=5, scoring=acc_scorer)
grid_obj = grid_obj.fit(x_train, y_train_binary)

# Set the clf to the best combination of parameters
clf = grid_obj.best_estimator_
```

Out[162]:
```
LogisticRegression(C=0.5, class_weight=None, dual=False, fit_interce
pt=True,
          intercept_scaling=1, max_iter=50, multi_class='ovr', n_job
s=1,
          penalty='l2', random_state=None, solver='liblinear', tol=0
.0001,
          verbose=0, warm_start=False)
```

In [163]:
```
train_test_model(clf, x_train, y_train_binary, x_test, y_test_binary)
```

```
              train      test
metrics
AUC        0.996631  0.998383
Accuracy   0.984925  0.988304
Precision  0.986395  0.984127
Recall     0.973154  0.984127
f1-score   0.979730  0.984127
```

Model II: Random forest

1. Random forest with all features

In [153]:
```
from sklearn.ensemble import RandomForestClassifier

# Choose some parameter combinations to try
parameters = {'n_estimators': 50,
              'max_features': 'auto',
              'criterion': 'gini',
              'max_depth': 20,
              'min_samples_split': 2,
              'min_samples_leaf': 20,
              'random_state': 0,
              'n_jobs': -1
              }

clf = RandomForestClassifier()

# Fit a model by providing X and y from training set
#clf.fit(x_train, y_train)



# Train test model
train_test_model(clf, x_train, y_train_binary, x_test, y_test_binary)
```

```
              train      test
metrics
AUC        0.999865  0.996032
Accuracy   0.992462  0.953216
Precision  0.986667  0.966102
Recall     0.993289  0.904762
f1-score   0.989967  0.934426
```

2. Random forest with hand-selected six features

In [156]:
```
clf = RandomForestClassifier()

train_test_train_test_model(clf, x_train_handSelected, y_train_binary,
x_test_handSelected, y_test_binary)model(clf, x_train_handSelected, y_
train_binary, x_test_handSelected, y_test_binary)
```

```
              train      test
metrics
AUC        0.999488  0.970018
Accuracy   0.997487  0.918129
Precision  1.000000  0.915254
Recall     0.993289  0.857143
f1-score   0.996633  0.885246
```

3. Random forest with cross validation & grid search

In [157]:
```
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import make_scorer, roc_auc_score, accuracy_score
from sklearn.model_selection import GridSearchCV

# Choose the type of classifier.
clf = RandomForestClassifier()

# Choose some parameter combinations to try
param_grid = {'n_estimators': [100,200],
              'max_features': ['auto'],
              'criterion': ['gini'],
              'max_depth': [15,20],
              'min_samples_split': [2],
              'min_samples_leaf': [2,10],
              'n_jobs':[-1]
             }

# Type of scoring used to compare parameter combinations
acc_scorer = make_scorer(roc_auc_score)

# Run the grid search
# read theory
grid_obj = GridSearchCV(clf, param_grid, cv=5, scoring=acc_scorer)
grid_obj = grid_obj.fit(_train, y_train)

# Set the clf to the best combination of parameters
clf = grid_obj.best_estimator_

# Fit the best algorithm to the data.
clf.fit(x_train, y_train)
```

Out[157]:
```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion=
'gini',
            max_depth=15, max_features='auto', max_leaf_nodes=None,
            min_impurity_decrease=0.0, min_impurity_split=None,
            min_samples_leaf=2, min_samples_split=2,
            min_weight_fraction_leaf=0.0, n_estimators=100, n_jobs=-
1,
            oob_score=False, random_state=None, verbose=0,
            warm_start=False)
```

In [159]:
```
train_test_model(clf, x_train_handSelected, y_train_binary, x_test_handSelected, y_test_binary)
```

```
                train      test
metrics
AUC         0.999407  0.978395
Accuracy    0.984925  0.912281
Precision   0.979866  0.875000
Recall      0.979866  0.888889
f1-score    0.979866  0.881890
```

Model comparison and conclusion

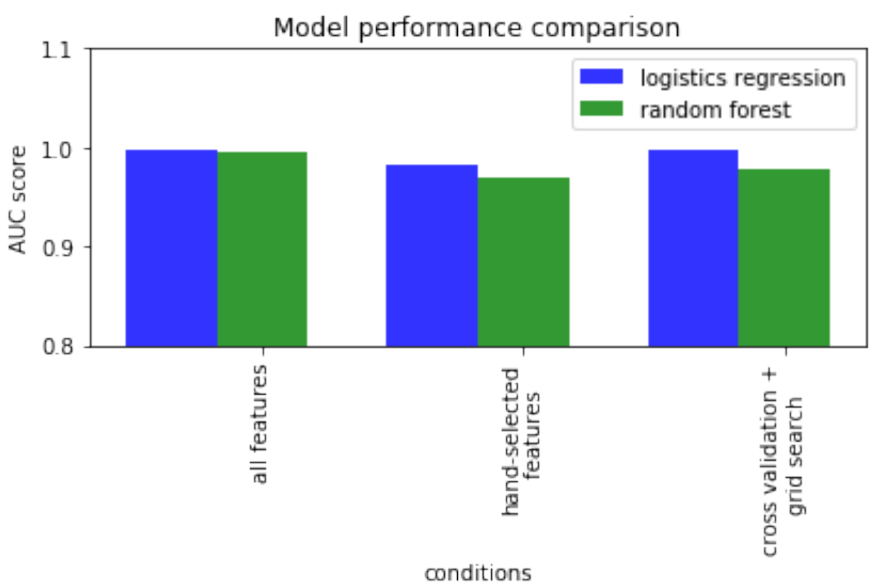
In [ ]:
```
## plot the performance of two methods
```

In [187]:
```
n_methods = 3
auc_log = (0.998089, 0.981922, 0.998383)
auc_ef = (0.996032, 0.970018, 0.978395)

bar_width = 0.35
opacity = 0.8

fig, ax = plt.subplots()
index - np.arange(n_methods)
plt.bar(index, auc_log, bar_width, alpha = opacity, color='b',label =
"logistics regression" )
plt.bar(index+bar_width, auc_ef, bar_width, alpha = opacity, color='g'
, label = "random forest" )
plt.xlabel('conditions')
plt.ylabel('AUC score')
plt.title('Model performance comparison')
plt.xticks(index + bar_width, ('all features', 'hand-selected\n
features', 'cross validation +\n grid search'), rotation=90)
plt.legend(loc=1)
plt.ylim(0.8,1.1)

plt.tight_layout()
plt.show()
```



- Both models achieve good performance (AUC>0.97) on all conditions
- In general, logistic regression perform bettern than random forest on this data set
- Reduce number of features lead to lower performance for both logistic regression and random forest