Using AI Tools to Identify Investment Candidates

Raymond Chiasson

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Approach – Build the Models

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Create training set of labeled drugs

Drug	Label
Vioxx	Good Drug
Mulresso	Good Drug
Zituxan	Bad Drug
DPN-15074	Bad Drug

+

2

Combined with key drug info from a drug database

Drug	Therapeutic Area	Indications	Designations	Sales 2018	Launch date	Summary
Zeyfalsda	Cancer; Infection	Acute myelogenous leukemia; Adenocarcinoma; Adenoid tumor; …	Accelerated Approval; Breakthrough Therapy; Orphan Drug;…	1022	Sept 2013	Merck & Co has developed and launched Zeyfalda with…

3

Build predictive models using AI tools

Drug	Label	Predicted Probability	Predicted Label
Vioxx	Good	97%	Good ✓
Mulresso	Good	70%	Good ✓
Zituxan	Bad	58%	Good ✗
DPN-15074	Bad	30%	Bad ✓

Approach – Screen Untested Drugs

Apply the models to untested drugs in database

+

~4,000 unscreened drugs marketed or in late-stage development

→

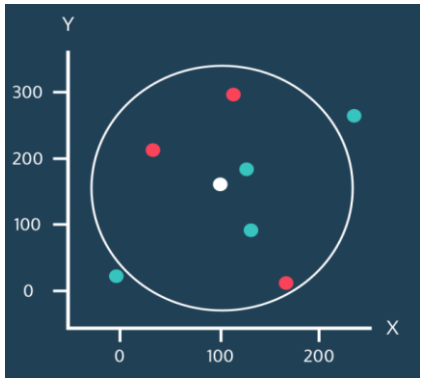
Identify most likely drug list candidates

Drug	Predicted probability
Varadolone	95%
RTX-5700	93%
Denilopan	93%
GTX-1650	88%

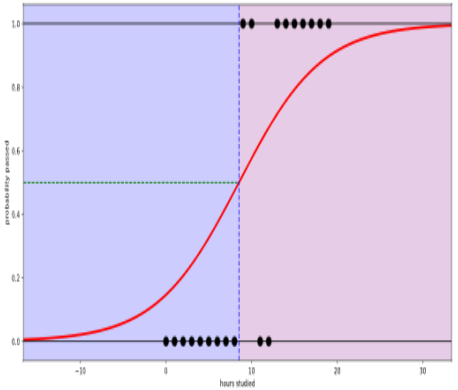
Building the Models – The Four Models

Algorithm	Description	Data types	Notes
K-nearest neighbors (KNN)	• Calculates the similarity (distance) between each point • Labels points according to the given for closest neighbors	• Numeric • Binary	• Little theoretical basis, but works well in practice • Computationally expensive
Logistical regression (LR)	• Linear regression mapped to a sigmoidal function so that results are between 0 and 1	• Numeric • Binary	• Well established technique • Can estimate impact of individual variables
Support vector machines (SVM)	• Draws a line between groups of data according to points nearest the boundary	• Numeric • Binary	• Conceptually simple • Computationally cheap
Naïve Bayes (Bayes)	• Labels based on word frequency and prior frequency of two labels	• Text	• Simple algorithm for text analysis • Famously used in spam filters

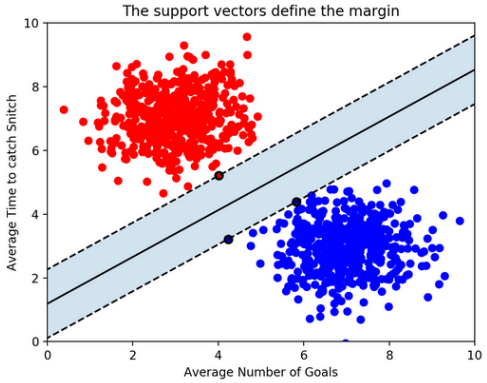
K-nearest neighbors



Logistical regression



Support Vector Machines



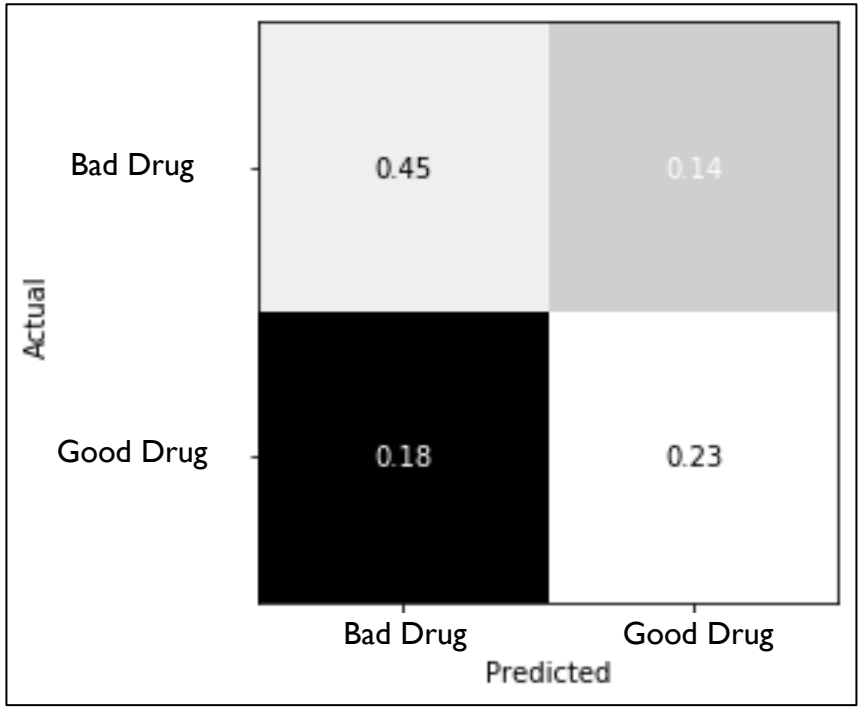
Naïve Bayes

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

	Percent Spam	Percent Not Spam
Urgent:	0.96	0.04
Urgent: limited	0.97	0.03
Urgent: limited time	0.81	0.19
Urgent: limited time offer	0.93	0.07

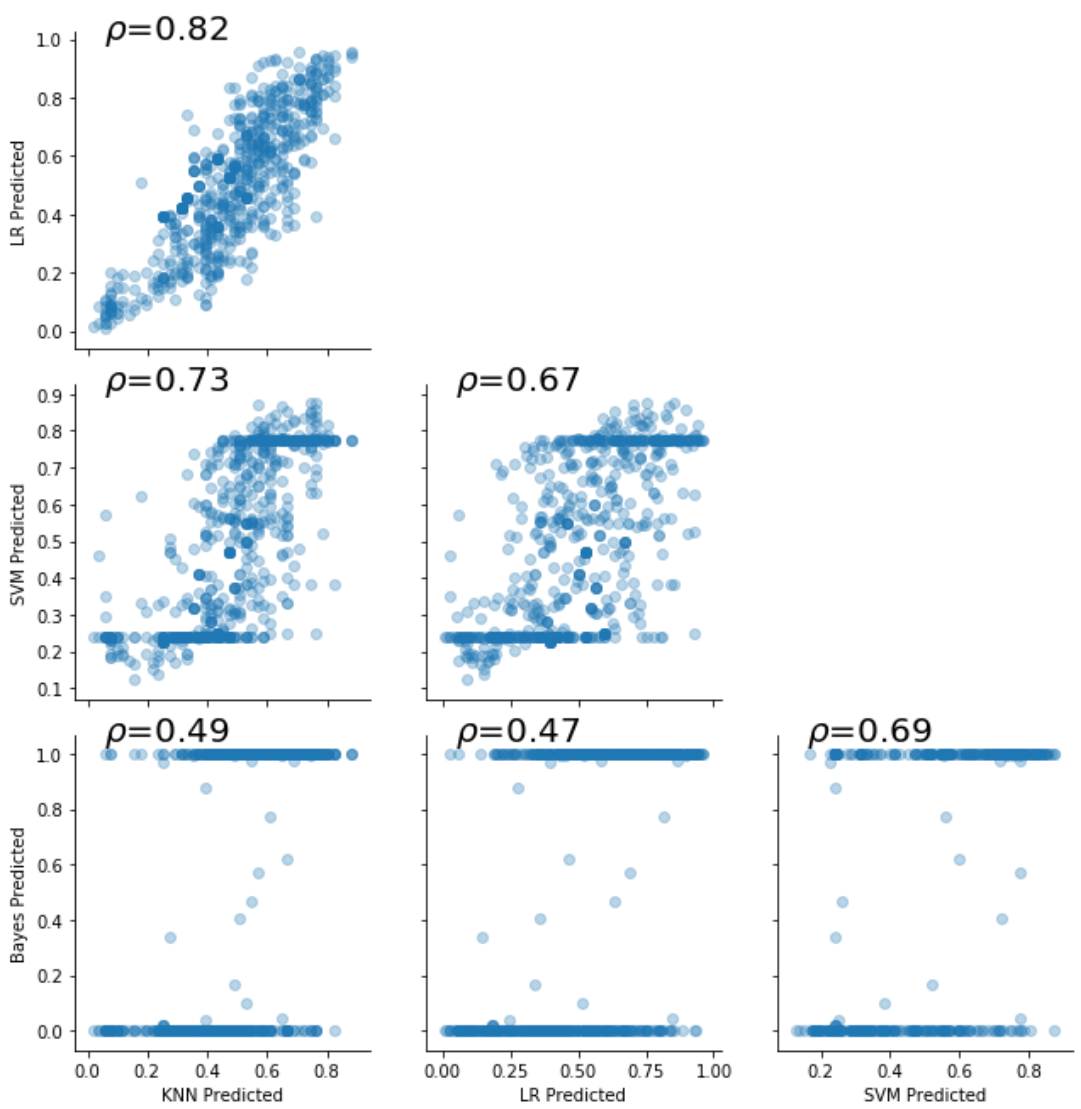
Building the Models - Sample code

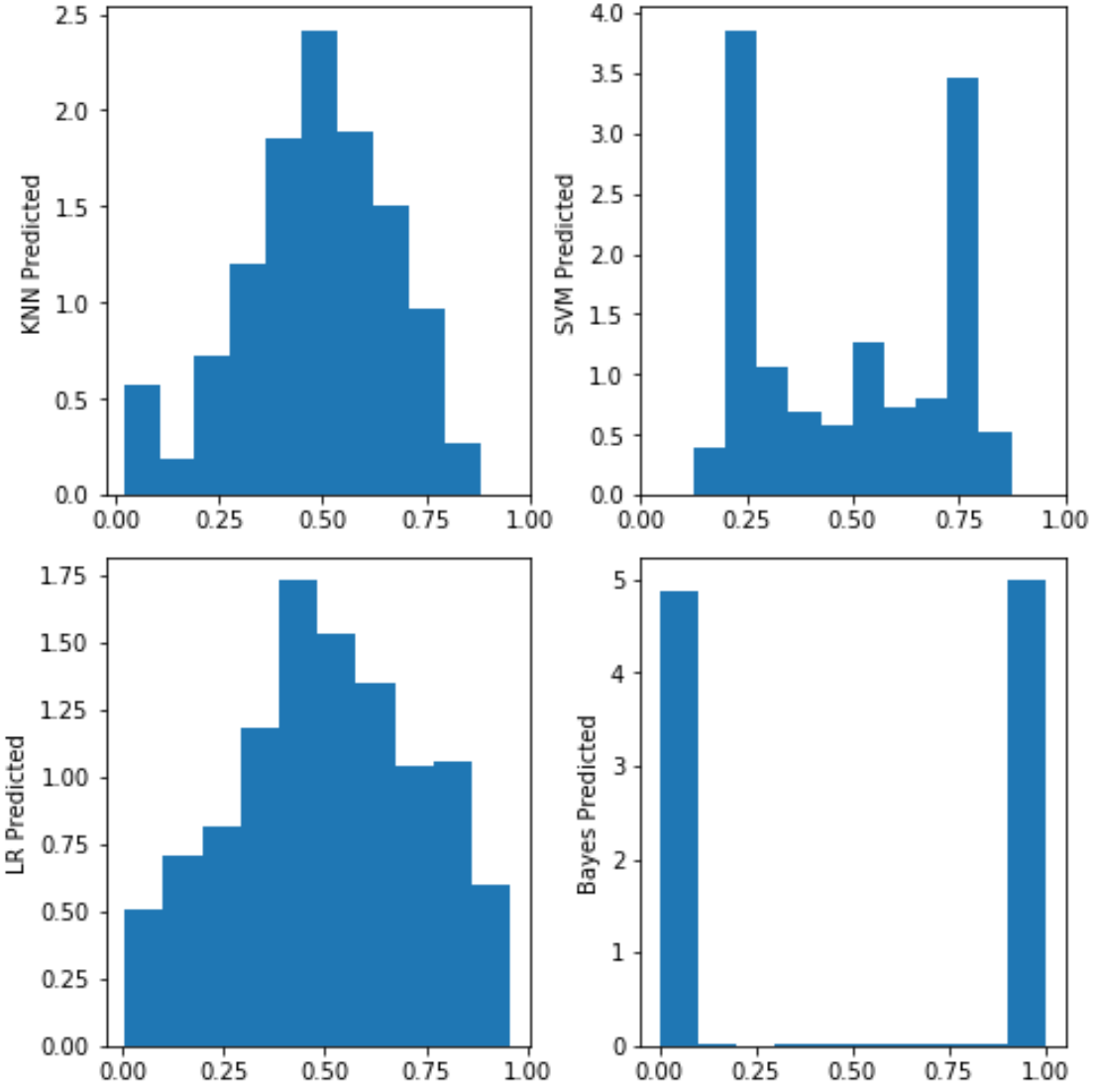
```
import pandas as pd
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import train_test_split
from sklearn import metrics
import matplotlib.pyplot as plt
import prep_and_analysis_functions as paf # custom analysis functions see file
from sklearn.model_selection import KFold

# load training set
training_set = pd.read_csv('training_set_standardized.csv')

'''
Part 1 - A - Prepare model for unapproved drugs
'''

#collect columns to input into model
feature_columns_unapproved = ['Fast_Track', 'SPA', 'Orphan', 'Breakthrough', 'RMAT', 'QIDP', 'large_public',
                  'small_public', 'phase_III_date_2015-2020', 'phase_III_date_2010-2014', 'phase_III_date_200
                  'Infectious disease', 'Psychiatry', 'Oncology', 'Autoimmune/immunology','Dermatology',
                  'Neurology', 'Respiratory', 'Endocrine', 'Hematology', 'Cardiovascular', 'Not Specified',
                  'Gastroenterology (non inflammatory bowel disease)', 'Obstetrics/Gynecology', 'Metabolic',
                  'Allergy', 'Ophthalmology', 'Urology', 'ENT/Dental', 'Renal', 'Orthopedics',
                  'Rheumatology (non autoimmune)', 'likelihood %', 'diff_from_avg']

# create features and labels list
features_unapproved = training_set.loc[training_set['approved']==0, feature_columns_unapproved]
labels_unapproved = training_set.loc[training_set['approved']==0, 'Drug List Status']

# build training/testing set
x_train, x_test, y_train, y_test = train_test_split(features_unapproved, labels_unapproved, test_size=0.2)

# create classifier object
knn_classifier = KNeighborsClassifier(n_neighbors=21) # see below for finding optimal value

# train model
knn_classifier.fit(x_train, y_train)
y_pred = knn_classifier.predict(x_test) # create predictions for test set

# quick accuracy check
paf.print_accuracy(y_test, y_pred)
paf.plot_confusion_matrix(y_test, y_pred)
paf.plot_confusion_matrix_normalized(y_test, y_pred)
```



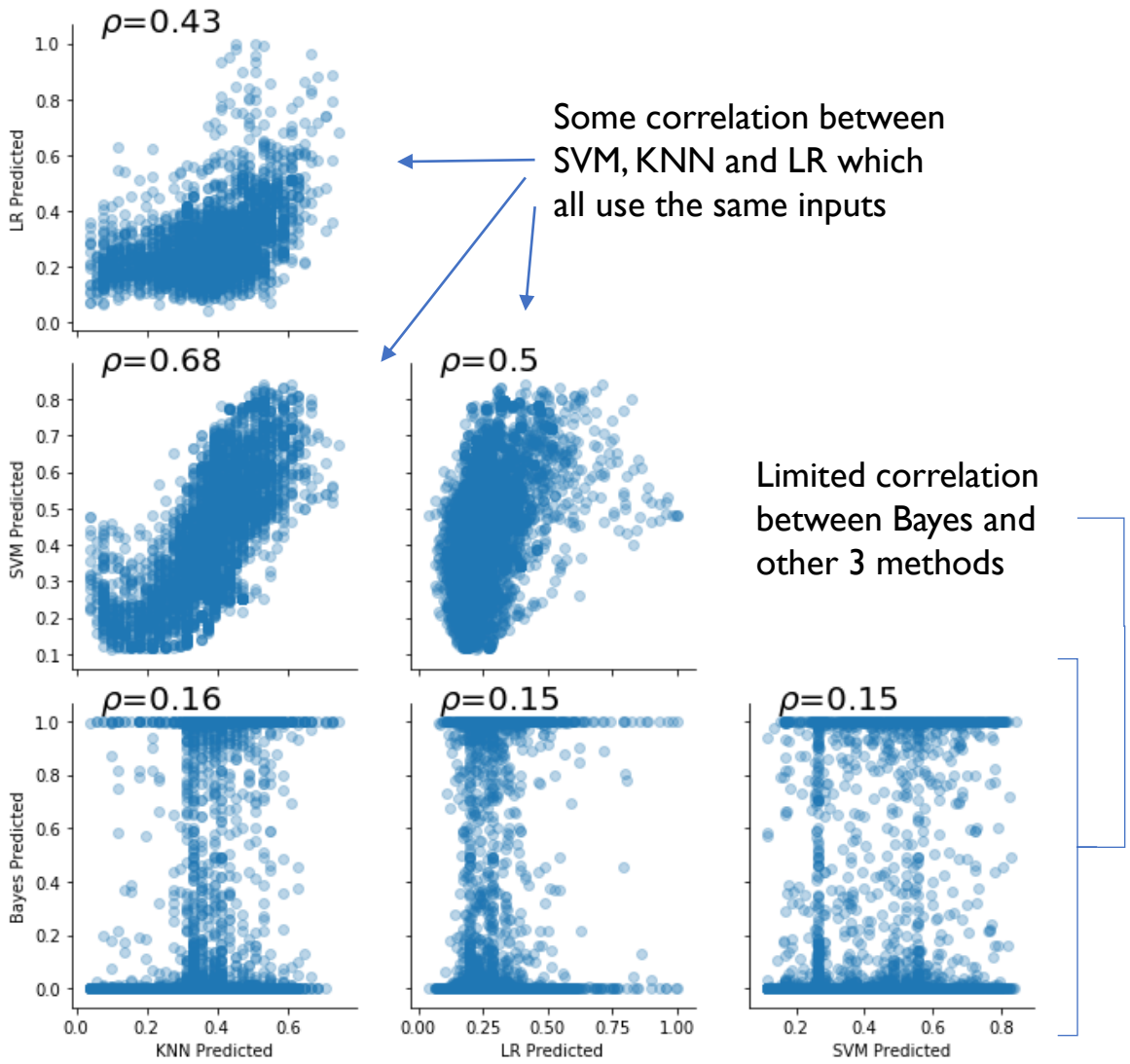

```
accuracy =  0.6785714285714286
recall =  0.5652173913043478
precision =  0.6190476190476191
f1 score =  0.5909090909090909
```

Building the Models - Model Correlation and Distribution (Training Set)





Applying the Models – Model Correlation and Distribution (testing set)



Some correlation between SVM, KNN and LR which all use the same inputs

Limited correlation between Bayes and other 3 methods