White_Vishwakarma_Project_2020

December 14, 2020

[479]:

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from adjustText import adjust_text
import synapseclient
from janitor import clean_names
import re
import string
import random
import collections
%matplotlib inline

## improve images
from IPython.display import set_matplotlib_formats, Image
set_matplotlib_formats('pdf', 'svg')
import json

#import rpy2.robjects as robjects
import rpy2.robjects as robjects
from rpy2.robjects import pandas2ri
pandas2ri.activate()

## sentiment analysis
from textblob import TextBlob
from nltk.sentiment.vader import SentimentIntensityAnalyzer
# nltk.download('vader_lexicon')
# from watson_developer_cloud import NaturalLanguageUnderstandingV1
# from watson_developer_cloud.natural_language_understanding_v1 import␣
 ↪Features, EntitiesOptions, KeywordsOptions, SentimentOptions,␣
 ↪CategoriesOptions

## text pre-processing
# nltk.download('punkt')
# nltk.download('stopwords')
# nltk.download('averaged_perceptron_tagger')
# nltk.download('wordnet')
```

```
import nltk
from word2number import w2n
import unidecode
import contractions
from nltk.corpus import stopwords
from nltk.corpus import wordnet
from wordcloud import WordCloud
from nltk.stem import WordNetLemmatizer
from sklearn.decomposition import PCA
from sklearn.feature_extraction.text import CountVectorizer
from sklearn.feature_extraction.text import TfidfVectorizer

## models
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LinearRegression
from sklearn.svm import SVR
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.model_selection import GridSearchCV

## metrics
from sklearn.neighbors import DistanceMetric
from sklearn.metrics import make_scorer
from sklearn.metrics import mean_squared_error
# from sklearn.metrics import f1_score
from sklearn.model_selection import cross_val_score

## Venn diagram package
from matplotlib_venn import venn3, venn3_circles

# import warnings
# warnings.filterwarnings('ignore')
```

[480]:

```
seed = 123
```

1 Import Data

[481]:

```
login = ''
pwd = ''
```

[482]:

```
syn = synapseclient.Synapse()
syn.login(login, pwd, rememberMe=True)
```

```
Welcome, Jess White!
```

1.1 Import Drug Screening Data

[483]:

```
#from Synapse-stored csv
drug_data_path = syn.get("syn20682897").path
data = pd.read_csv(drug_data_path, low_memory=False)

#from Synapse table
results = syn.tableQuery("SELECT * FROM syn20556247")
data = results.asDataFrame()
```

```
[WARNING] C:\Users\jessb\anaconda3\lib\site-
packages\IPython\core\interactiveshell.py:3343: DtypeWarning: Columns (10) have
mixed types.Specify dtype option on import or set low_memory=False.
```

[159]:

```
## saved as csv file in case we lose access
# compression_opts = dict(method='zip',
#                         archive_name='out.csv')

# data.to_csv('../assets/out.zip',
#             compression=compression_opts, index=False)
```

1.2 Elsevier Data

[ ]:

```
# df_journal = pd.read_json(syn.get("syn22797452").path, lines=True)

with open('../assets/elsevier/ctf-hackathon-upload.json',␣
 ↪encoding='iso-8859-1') as f:
  df_journal = json.load(f)
```

1.3 Drug Annotations

1.3.1 Drug Target Explorer Data

[503]:

```
targetspath = syn.get('syn17091507')
readRDS = robjects.r['readRDS']

df_drugs = readRDS(targetspath.path)
```

[504]:

```
df_drugs.columns
```

[504]:

```
Index(['internal_id', 'hugo_gene', 'n_quantitative', 'mean_pchembl', 'cv',
       'sd', 'IC50_nM', 'AC50_nM', 'EC50_nM', 'Potency_nM', 'Ki_nM', 'Kd_nM',
       'n_qualitative', 'std_name', 'total_n', 'confidence', 'pchembl_d',
       'pchembl_t', 'known_selectivity_index'],
      dtype='object')
```

[505]:

```
## tutorial suggests defining real MOA as mean_pchembl > 6
df_drugs_moa = (df_drugs
                .query('mean_pchembl > 6')
                .filter(["internal_id", "hugo_gene", "std_name"])
                .drop_duplicates())

df_drugs_moa.head()
```

[505]:

```
   internal_id hugo_gene       std_name
1            3      HTR7  CHEMBL2413451
2            4    CHRNA4   CHEMBL204871
3            4    CHRNB2   CHEMBL204871
4            5     GSK3A  CHEMBL3582401
5            6      FAAH  CHEMBL2386554
```

1.3.2 Thesis Annotations

[508]:

```
df_moa = pd.read_csv('../assets/moa.csv', header=0)
```

[509]:

```
## replace - with ""
df_moa.Drugs = df_moa.Drugs.replace("-", "", regex = True)
## set all values lower case
df_moa.Drugs = df_moa.Drugs.str.lower()

# df_moa = df_moa.drop_duplicates()
```

2 Drug Screening Data Prep

2.1 Drug Screening EDA

[510]:

```
data.head()
```

[510]:

```
             data_contributor  data_contact  drug_screen_id   drug_assay_id  \
5010113_3768              UMN       3335875               1  syn11373153.17
5010114_3768              UMN       3335875               1  syn11373153.18
5010115_3768              UMN       3335875               1  syn11373153.19
5010116_3768              UMN       3335875               1  syn11373153.20
5010117_3768              UMN       3335875               1  syn11373153.21

             experiment_synapse_id study_synapse_id funder model_name  \
5010113_3768         syn11373153.1       syn5610425    CTF        N10
5010114_3768         syn11373153.1       syn5610425    CTF        N10
5010115_3768         syn11373153.1       syn5610425    CTF        N10
5010116_3768         syn11373153.1       syn5610425    CTF        N10
5010117_3768         syn11373153.1       syn5610425    CTF        N10
```

```
             cellosaurus_id organism_name  …      dosage  dosage_unit  \
5010113_3768            NaN         human  …  100.000000           uM
5010114_3768            NaN         human  …   33.333430           uM
5010115_3768            NaN         human  …   11.111175           uM
5010116_3768            NaN         human  …    3.703736           uM
5010117_3768            NaN         human  …    1.234554           uM

                response      response_type  response_unit model_type  \
5010113_3768   99.979123  percent viability              %  cell line
5010114_3768  103.789330  percent viability              %  cell line
5010115_3768  102.178887  percent viability              %  cell line
5010116_3768  104.653527  percent viability              %  cell line
5010117_3768  105.312040  percent viability              %  cell line

             disease_name disease_efo_id symptom_name  symptom_efo_id
5010113_3768   no disease            NaN   no symptom             NaN
5010114_3768   no disease            NaN   no symptom             NaN
5010115_3768   no disease            NaN   no symptom             NaN
5010116_3768   no disease            NaN   no symptom             NaN
5010117_3768   no disease            NaN   no symptom             NaN

[5 rows x 22 columns]
```

```
[511]: data.shape
```

```
[511]: (928480, 22)
```

```
[512]: col_list = data.columns.to_list()

       for n in col_list:
           print(n)
           print(data[n].value_counts())
           print()
```

```
data_contributor
NCATS    881838
UCF       22174
UMN       21408
MGH        3060
Name: data_contributor, dtype: int64

data_contact
3334155    881838
3334459     22174
3335875     21408
3321266      3060
Name: data_contact, dtype: int64
```

```
drug_screen_id
41423    576
17131    360
21640    360
21437    360
19371    360
        …
41312     10
41313     10
41314     10
41308     10
41311     10
Name: drug_screen_id, Length: 43371, dtype: int64
```

```
drug_assay_id
syn18457441.30527    2
syn18457466.32789    2
syn18457441.29053    2
syn18457474.2097     2
syn18457441.10689    2
                    ..
syn6138251.9182      1
syn12293957.18812    1
syn5522642.2024      1
syn12293963.20556    1
syn6138251.12414     1
Name: drug_assay_id, Length: 689680, dtype: int64
```

```
experiment_synapse_id
syn18457448.1    56760
syn18457441.1    56760
syn18457466.1    56760
syn18457456.1    56760
syn6138251.1     25234
                 …
syn11373167.1       32
syn11373414.1       32
syn11373541.1       32
syn11373334.1       32
syn11373700.1       32
Name: experiment_synapse_id, Length: 711, dtype: int64
```

```
study_synapse_id
syn2343195    675720
syn4939906    231352
syn5610425     21408
Name: study_synapse_id, dtype: int64
```

```
funder
CTF     697128
NTAP    231352
Name: funder, dtype: int64

model_name
Syn5                       163759
Syn1                       142727
HS11                       142160
HS01                       142160
Ben-Men-1                   42404
MS02                        26504
ipNF05.5 (single clone)     21032
ipn02.3                     21032
ipNF95.11b C                21032
ipNF95.6                    21032
ipNF05.5 (mixed clone)      21032
ipNF95.11b C/T              21032
MTC                         21032
ipNF06.2A                   21032
HFF                         21032
ipnNF95.11C                 21032
ipn02.8                     21032
N10                         10704
N5                          10704
MS11                         5760
MS01                         5470
MS12                         1368
MS03                         1368
Syn12                         340
Syn3                          340
Syn10                         340
Syn2                          340
Syn4                          340
Syn7                          340
Name: model_name, dtype: int64

cellosaurus_id
CVCL_1959    42404
Name: cellosaurus_id, dtype: int64

organism_name
human    866978
mouse     61502
Name: organism_name, dtype: int64

drug_name
```

```
NCGC00351602-01    21022
NCGC00378921-01    16680
NCGC00250408-01    14729
NCGC00263203-01    14542
NCGC00346931-02    14520
                   …
NCGC00386425-06       22
NCGC00356417-01       22
NCGC00351604-01       22
NCGC00378588-02       22
NCGC00273985-01       22
Name: drug_name, Length: 2722, dtype: int64

DT_explorer_internal_id
191922    21022
313781    18862
98169     17609
79046     16702
251077    16191
          …
313764       22
313176       22
313824       22
189206       22
146370       22
Name: DT_explorer_internal_id, Length: 2424, dtype: int64

dosage
5.000000e+00    28322
4.608295e+01    18798
5.689253e-01    18530
6.321392e-02    18530
2.341244e-03    18530
                …
2.730000e-07        1
7.370000e-06        1
5.270000e-09        1
2.720000e-05        1
1.010000e-06        1
Name: dosage, Length: 504, dtype: int64

dosage_unit
uM    928480
Name: dosage_unit, dtype: int64

response
0.000000      698
100.000000     15
```

```
0.460435        6
0.438770        6
1.330835        6
             …
93.349130       1
112.768735      1
112.738448      1
65.550671       1
106.560431      1
Name: response, Length: 687047, dtype: int64

response_type
percent viability    928480
Name: response_type, dtype: int64

response_unit
%    928480
Name: response_unit, dtype: int64

model_type
cell line    928480
Name: model_type, dtype: int64

disease_name
no disease    387187
NF2           383365
NF1           157928
Name: disease_name, dtype: int64

disease_efo_id
Series([], Name: disease_efo_id, dtype: int64)

symptom_name
no symptom    704490
pNF           147224
meningioma     43424
schwannoma     33342
Name: symptom_name, dtype: int64

symptom_efo_id
693.0    175502
658.0    147224
Name: symptom_efo_id, dtype: int64
```

```
[513]: data.apply(lambda x: sum(x.isnull()), axis=0)
```

[513]:

```
data_contributor                0
data_contact                    0
drug_screen_id                  0
drug_assay_id                   0
experiment_synapse_id           0
study_synapse_id                0
funder                          0
model_name                      0
cellosaurus_id             886076
organism_name                   0
drug_name                       0
DT_explorer_internal_id         0
dosage                          0
dosage_unit                     0
response                        0
response_type                   0
response_unit                   0
model_type                      0
disease_name                    0
disease_efo_id             928480
symptom_name                    0
symptom_efo_id             605754
dtype: int64
```

[514]:

```
data.dtypes
```

[514]:

```
data_contributor            object
data_contact                 int64
drug_screen_id               int64
drug_assay_id               object
experiment_synapse_id       object
study_synapse_id            object
funder                      object
model_name                  object
cellosaurus_id              object
organism_name               object
drug_name                   object
DT_explorer_internal_id      int64
dosage                     float64
dosage_unit                 object
response                   float64
response_type               object
response_unit               object
model_type                  object
disease_name                object
disease_efo_id             float64
symptom_name                object
```

```
symptom_efo_id              float64
dtype: object
```

[515]:

```
print(data[(data.symptom_name == 'meningioma')].disease_name.value_counts())
print()
print(data[(data.symptom_name == 'schwannoma')].disease_name.value_counts())
print()
print(data[(data.symptom_name == 'pNF')].disease_name.value_counts())
print()
print(data[(data.symptom_name == 'no symptom')].disease_name.value_counts())
```

```
NF2    43424
Name: disease_name, dtype: int64

NF2    33342
Name: disease_name, dtype: int64

NF1    147224
Name: disease_name, dtype: int64

no disease    387187
NF2           306599
NF1            10704
Name: disease_name, dtype: int64
```

[516]:

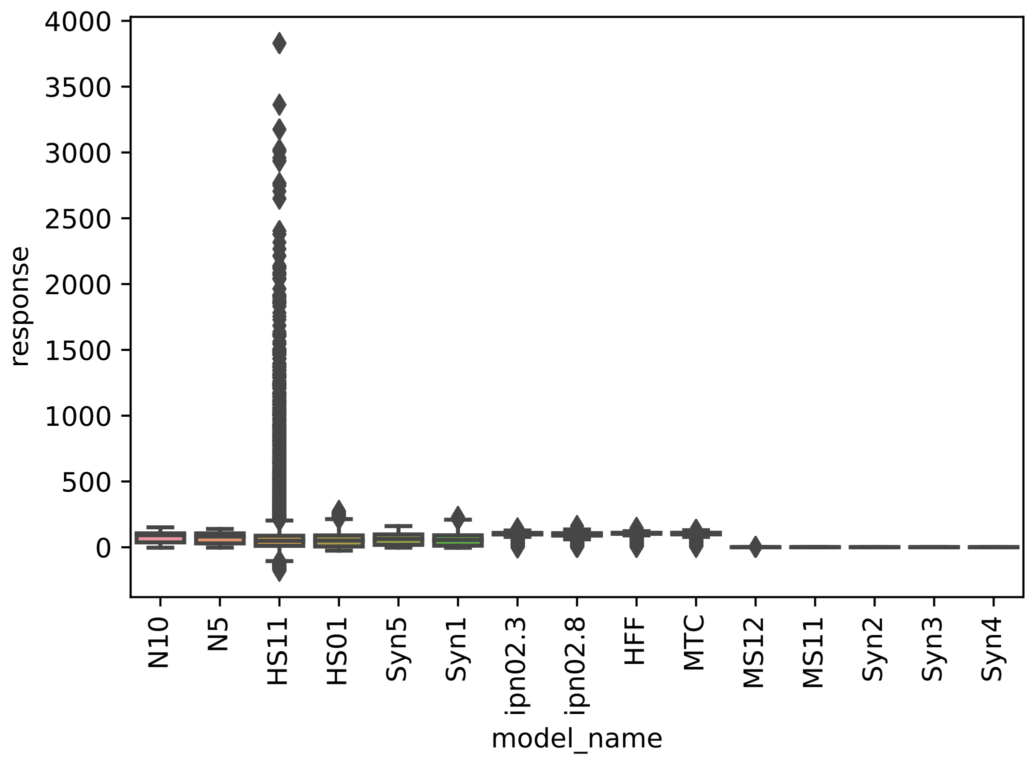
```
set(data.model_name.loc[((data.symptom_name == 'meningioma')|
                          (data.symptom_name == 'schwannoma')|
                          (data.symptom_name == 'pNF'))])
```

[516]:

```
{'Ben-Men-1',
 'MS01',
 'MS02',
 'MS03',
 'Syn10',
 'Syn12',
 'Syn7',
 'ipNF05.5 (mixed clone)',
 'ipNF05.5 (single clone)',
 'ipNF06.2A',
 'ipNF95.11b C',
 'ipNF95.11b C/T',
 'ipNF95.6',
 'ipnNF95.11C'}
```

[518]:

```
ax = sns.boxplot(x = 'model_name', y = 'response',
                 data = data.loc[(data.symptom_name == 'no symptom')]);
ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);
```



2.2 Drug Screening Pre-Processing

[519]:

```
## dosage unit all micromolar
## respose type all percent viability
## response unit all %
## model type all cell line
## cellosaurus_id, disease_efo_id, symptom_efo_id
## contain a lot of missing data and no key

drop_list = ['dosage_unit', 'response_type', 'response_unit',
             'model_type', 'disease_efo_id', 'symptom_efo_id',
             'cellosaurus_id']

data.drop(columns = drop_list, inplace = True)
```

[520]:

```
## df_drugs contains duplicates (ordered by MOA)
## keep only internal_id and std_name for mapping
df_drug_min = df_drugs.loc[:, ['internal_id', 'std_name']]
df_drug_min.drop_duplicates(inplace=True)

print(df_drug_min.shape)
print(len(set(df_drug_min.internal_id)))
print(len(set(df_drug_min.std_name)))

data = data.merge(df_drug_min,
                  left_on = "DT_explorer_internal_id",
                  right_on = "internal_id",
                  how = "inner")
```

```
(305219, 2)
305219
305219
```

Looks like some % viability expressed as integers and others as %. HS11 seems like an outlier even when adjusting so dropped those rows.

[521]:

```
## drop HS11 cell line
## too high to be merely integer viability
data = data[(data.model_name != 'HS11')]
```

[522]:

```
set(data.model_name)
```

[522]:

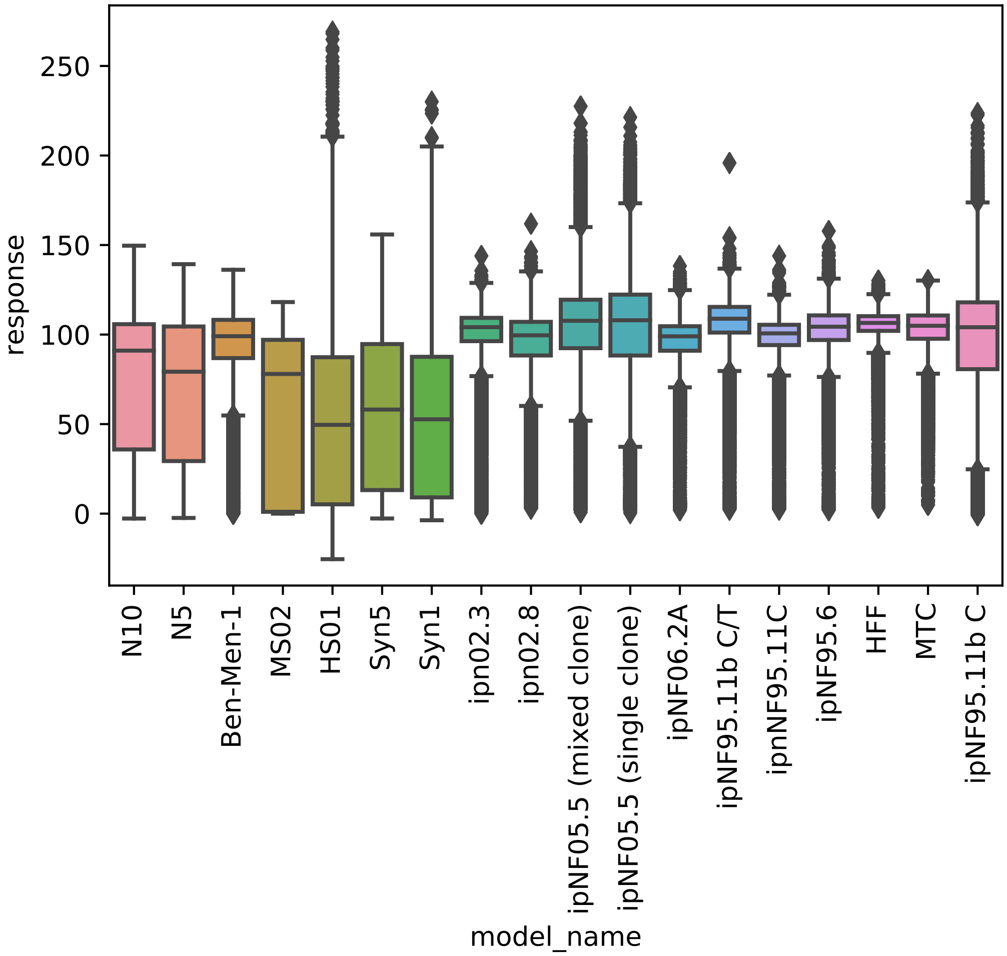
```
{'Ben-Men-1',
 'HFF',
 'HS01',
 'MS01',
 'MS02',
 'MS03',
 'MS11',
 'MS12',
 'MTC',
 'N10',
 'N5',
 'Syn1',
 'Syn10',
 'Syn12',
 'Syn2',
 'Syn3',
 'Syn4',
 'Syn5',
 'Syn7',
 'ipNF05.5 (mixed clone)',
 'ipNF05.5 (single clone)',
 'ipNF06.2A',
 'ipNF95.11b C',
 'ipNF95.11b C/T',
 'ipNF95.6',
 'ipn02.3',
 'ipn02.8',
 'ipnNF95.11C'}
```

[523]:

```
## cell lines where viability expressed as integer instead of %
scale_list = ['Ben-Men-1', 'MS02', 'ipNF05.5 (mixed clone)', 'ipNF05.5 (single␣
 ↪clone)',
               'ipNF06.2A', 'ipNF95.11b C', 'ipNF95.11b C/T', 'ipNF95.6',␣
 ↪'ipnNF95.11C',
               'N10', 'N5', 'HS01', 'Syn1', 'Syn5', 'ipn02.3', 'ipn02.8', 'HFF',␣
 ↪'MTC']
```

[524]:

```
# check that the integer scaled to percent are not outliers
ax = sns.boxplot(x = 'model_name', y = 'response',
                 data = data.loc[(data.model_name.apply(lambda x: x in␣
 ↪scale_list))]);
ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);
```

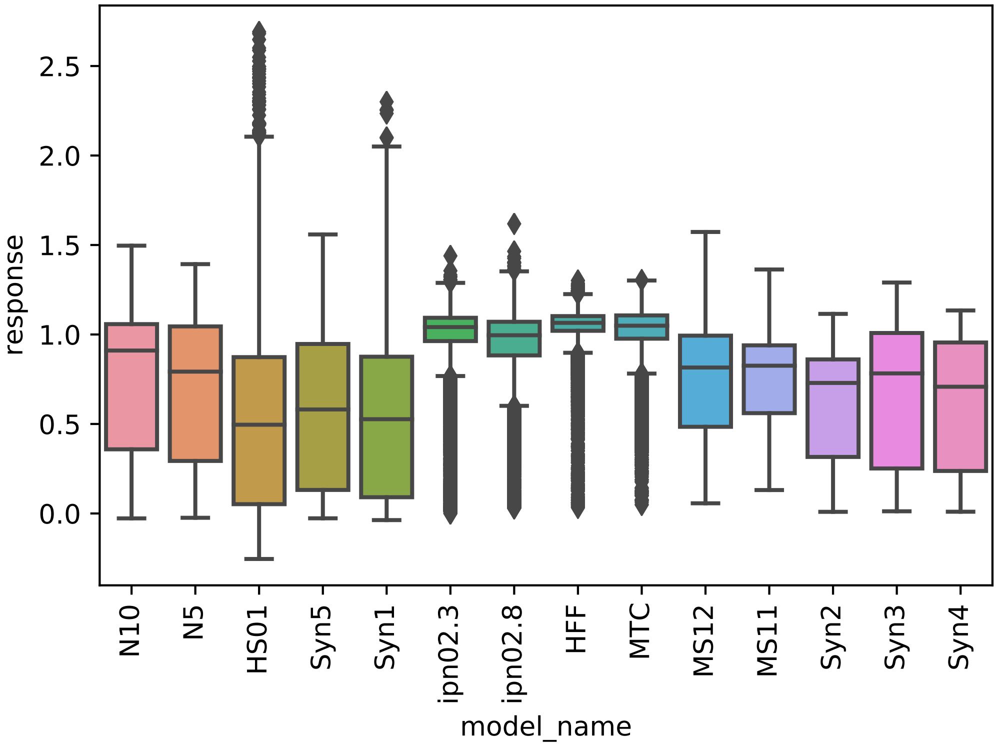


[525]:

```
## replace integer values with percentage
data.loc[(data.model_name.apply(lambda x: x in scale_list)), "response"] =\
    data.loc[(data.model_name.apply(lambda x: x in scale_list)), "response"]/100
```

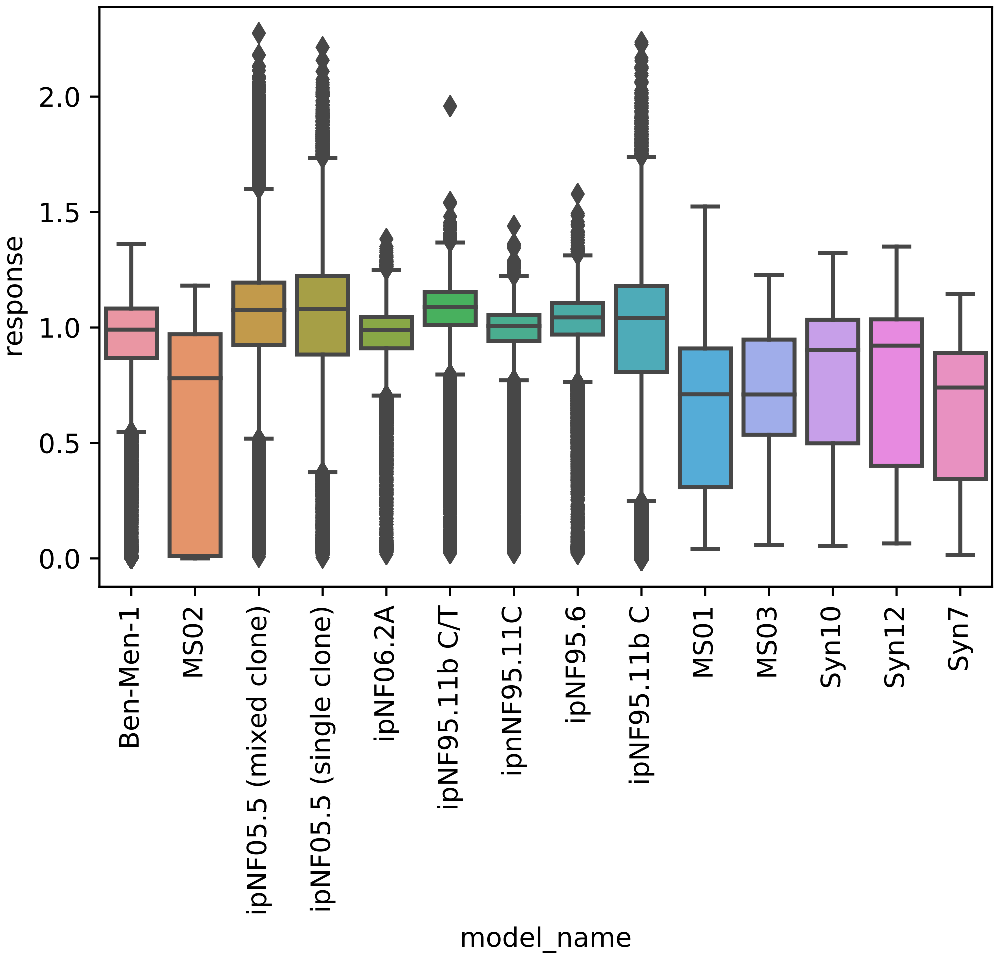
[526]:

```
## for no symptom cell lines
ax = sns.boxplot(x = 'model_name', y = 'response',
                 data = data.loc[(data.symptom_name == 'no symptom')]);
ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);
```



[527]:

```
## for disease cell lines
ax = sns.boxplot(x = 'model_name', y = 'response',
                 data = data.loc[((data.symptom_name == 'meningioma')|
                                  (data.symptom_name == 'schwannoma')|
                                 (data.symptom_name == 'pNF'))]);
ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);
```



[528]:

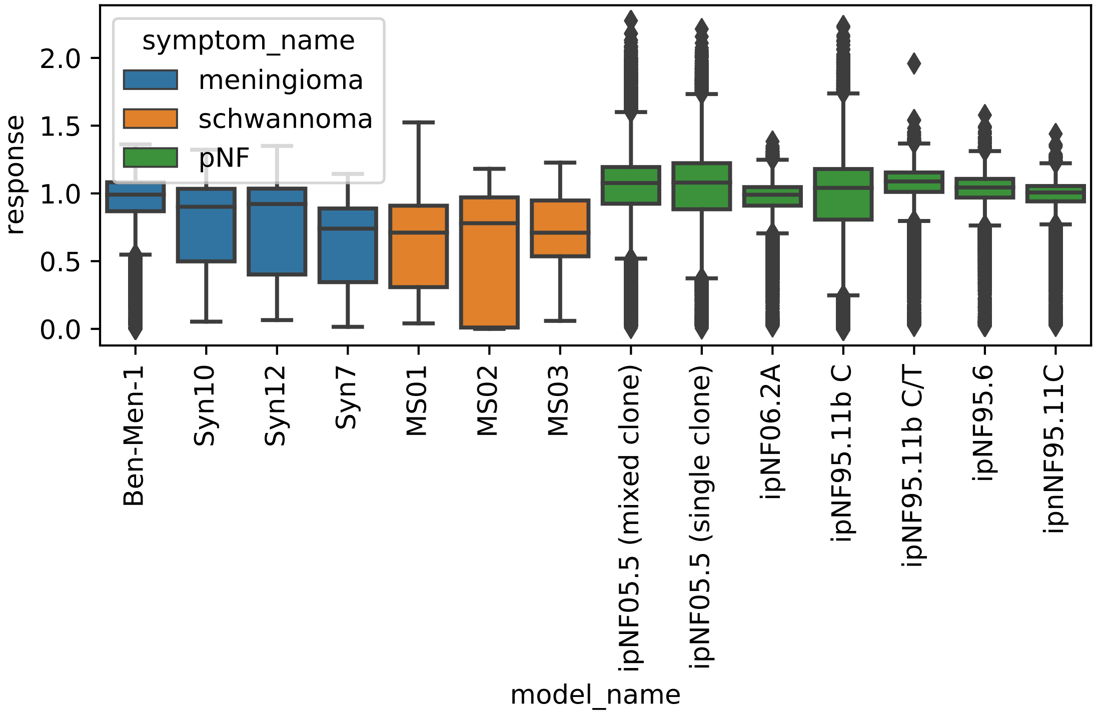
```python
## extract only cell line,symptom, and disease
## remove repeats and store in single dataframe
df_cell_disease = data.loc[:, ['model_name', 'symptom_name', 'disease_name']]
df_cell_disease.drop_duplicates(inplace=True)
df_cell_disease.reset_index(inplace=True)
df_cell_disease.head()
```

[528]:

```
   index model_name symptom_name disease_name
0      0        N10   no symptom   no disease
1     16         N5   no symptom          NF1
2     32  Ben-Men-1   meningioma          NF2
3     43       MS02   schwannoma          NF2
4     65       HS01   no symptom          NF2
```

[529]:

```python
ax = sns.boxplot(x = 'model_name', y = 'response', hue = 'symptom_name',
                 data = data.loc[((data.symptom_name == 'meningioma')|
                                  (data.symptom_name == 'schwannoma')|
                                 (data.symptom_name == 'pNF'))],
                 order=['Ben-Men-1', 'Syn10', 'Syn12', 'Syn7',
                        'MS01', 'MS02', 'MS03',
                        'ipNF05.5 (mixed clone)', 'ipNF05.5 (single clone)',
                        'ipNF06.2A', 'ipNF95.11b C', 'ipNF95.11b C/T',
                        'ipNF95.6', 'ipnNF95.11C'],
                 dodge=False);
ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);

plt.tight_layout()
plt.savefig("../images/Fig2.png", dpi=410)
```



2.3 MEK inhibitor comparison

[530]:
```
df_mek = data[((data.std_name.str.lower() == 'selumetinib') |
               (data.std_name.str.lower() == 'trametinib') |
               (data.std_name.str.lower() == 'binimetinib') |
               (data.std_name.str.lower() == 'pd-0325901'))]

df_mek = df_mek[(data.symptom_name == 'pNF')]

df_mek.loc[:, 'std_name'] = df_mek.std_name.astype('string')
df_mek.std_name.value_counts()
```

```
[WARNING] <ipython-input-530-0f326f05a618>:6: UserWarning: Boolean Series key
will be reindexed to match DataFrame index.
```

[530]:

```
SELUMETINIB    77
BINIMETINIB    77
PD-0325901     77
TRAMETINIB     77
Name: std_name, dtype: Int64
```

[531]:

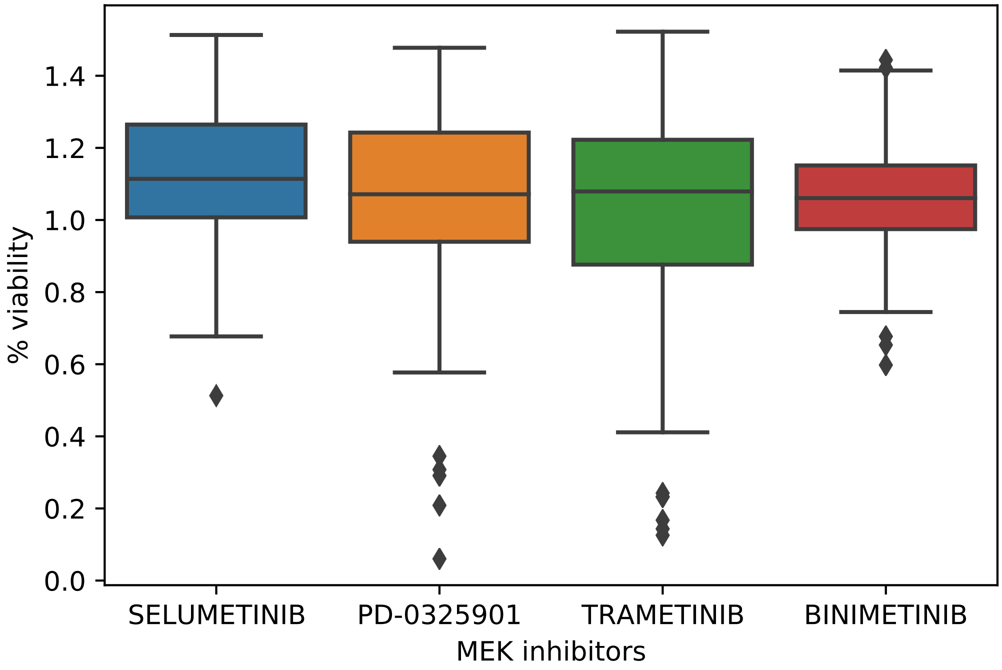
```
df_mek.symptom_name.value_counts()
```

[531]:

```
pNF    308
Name: symptom_name, dtype: int64
```

[532]:

```
sns.boxplot(x = 'std_name', y = 'response', data = df_mek);
plt.xlabel('MEK inhibitors');
plt.ylabel('% viability');
plt.savefig("../images/Fig3.png", dpi=410);
```



2.3.1 Summary by Cell Line

[ ]:

```
## will take a while to run
data_cell_median = (data
                    .groupby('std_name').filter(lambda x: len(x)>3)
                    .filter(['std_name', 'response','model_name'])
                    .groupby(['std_name','model_name'],as_index = False).
 ↪median())

data_cell_mean = (data
                  .groupby('std_name').filter(lambda x: len(x)>3)
                  .filter(['std_name', 'response','model_name'])
                  .groupby(['std_name','model_name'],as_index = False).mean())

data_cell_min = (data
                 .groupby('std_name').filter(lambda x: len(x)>3)
                 .filter(['std_name', 'response','model_name'])
                 .groupby(['std_name','model_name'],as_index = False).min())

data_cell_max = (data
                 .groupby('std_name').filter(lambda x: len(x)>3)
                 .filter(['std_name', 'response','model_name'])
                 .groupby(['std_name','model_name'],as_index = False).max())

data_cell_median.dropna(axis=0, inplace=True)
data_cell_mean.dropna(axis=0, inplace=True)
data_cell_min.dropna(axis=0, inplace=True)
data_cell_max.dropna(axis=0, inplace=True)

data_cell_median.rename(columns={'response':'median'}, inplace=True)
data_cell_mean.rename(columns={'response':'mean'}, inplace=True)
data_cell_min.rename(columns={'response':'min'}, inplace=True)
data_cell_max.rename(columns={'response':'max'}, inplace=True)

print(data_cell_median.shape)
print(data_cell_mean.shape)
print(data_cell_min.shape)
print(data_cell_max.shape)
```

[35]:

```
data_cell_summary = data_cell_median.merge(data_cell_mean,
                                           left_on = ['std_name', 'model_name'],
                                           right_on = ['std_name',␣
 ↪'model_name'],
                                           how = "inner")

data_cell_summary = data_cell_summary.merge(data_cell_min,
                                             left_on = ['std_name',␣
↪'model_name'],
                                             right_on = ['std_name',␣
↪'model_name'],
                                             how = "inner")

data_cell_summary = data_cell_summary.merge(data_cell_max,
                                             left_on = ['std_name',␣
↪'model_name'],
                                             right_on = ['std_name',␣
↪'model_name'],
                                             how = "inner")

print(data_cell_summary.shape)
data_cell_summary.head()
```

```
(19094, 6)
```

[35]:

```
                   std_name model_name    median      mean       min       max
0  (-)-Deoxypodophyllotoxin        N10  0.600546  0.694651  0.479870  1.162219
1  (-)-Deoxypodophyllotoxin         N5  0.398599  0.548063  0.328342  1.284884
2         (-)-Gambogic Acid        N10  0.368344  0.506716 -0.008534  1.130643
3         (-)-Gambogic Acid         N5  0.412480  0.453455 -0.007143  0.966614
4         (-)-NORADRENALINE  Ben-Men-1  0.893658  0.884852  0.741394  1.023629
```

[410]:

```
## https://towardsdatascience.com/
↪name-your-favorite-excel-function-and-ill-teach-you-its-pandas-equivalent-7ee4400ada9f
data_cell_summary['disease_name'] = \
    data_cell_summary.model_name.map(df_cell_disease.
↪set_index('model_name')['disease_name'].to_dict())
data_cell_summary['symptom_name'] = \
    data_cell_summary.model_name.map(df_cell_disease.
↪set_index('model_name')['symptom_name'].to_dict())

data_cell_summary.head()
```

[410]:

```
                   std_name model_name    median      mean       min  \
0  (-)-Deoxypodophyllotoxin        N10  0.600546  0.694651  0.479870
1  (-)-Deoxypodophyllotoxin         N5  0.398599  0.548063  0.328342
2         (-)-Gambogic Acid        N10  0.368344  0.506716 -0.008534
3         (-)-Gambogic Acid         N5  0.412480  0.453455 -0.007143
4         (-)-NORADRENALINE  Ben-Men-1  0.893658  0.884852  0.741394

        max disease_name symptom_name
0  1.162219   no disease   no symptom
1  1.284884          NF1   no symptom
2  1.130643   no disease   no symptom
```

```
3  0.966614          NF1   no symptom
4  1.023629          NF2   meningioma
```

[366]:

```
print(data_cell_summary.dtypes)
data_cell_summary['std_name'] = data_cell_summary.std_name.astype(str)
```

```
std_name        category
model_name        object
median           float64
mean             float64
min              float64
max              float64
disease_name      object
dtype: object
```

[411]:

```
# saved as csv file since takes some time to run
# compression_opts = dict(method='zip',
#                         archive_name='out.csv')

data_cell_summary.to_csv('../assets/data_cell_summary.csv', index=False)
#             compression=compression_opts)
```

2.3.2 Summary by Disease

[236]:

```
## will take a while to run
data_disease_median = (data
                       .groupby('std_name').filter(lambda x: len(x)>3)
                       .filter(['std_name', 'response','symptom_name'])
                       .groupby(['std_name','symptom_name'],as_index = False).
 ↪median())

data_disease_mean = (data
                     .groupby('std_name').filter(lambda x: len(x)>3)
                     .filter(['std_name', 'response','symptom_name'])
                     .groupby(['std_name','symptom_name'],as_index = False).
 ↪mean())

data_disease_min = (data
                    .groupby('std_name').filter(lambda x: len(x)>3)
                    .filter(['std_name', 'response','symptom_name'])
                    .groupby(['std_name','symptom_name'],as_index = False).
 ↪min())

data_disease_max = (data
                    .groupby('std_name').filter(lambda x: len(x)>3)
                    .filter(['std_name', 'response','symptom_name'])
                    .groupby(['std_name','symptom_name'],as_index = False).
 ↪max())

data_disease_median.dropna(axis=0, inplace=True)
data_disease_mean.dropna(axis=0, inplace=True)
data_disease_min.dropna(axis=0, inplace=True)
data_disease_max.dropna(axis=0, inplace=True)

data_disease_median.rename(columns={'response':'median'}, inplace=True)
data_disease_mean.rename(columns={'response':'mean'}, inplace=True)
data_disease_min.rename(columns={'response':'min'}, inplace=True)
data_disease_max.rename(columns={'response':'max'}, inplace=True)

print(data_disease_median.shape)
print(data_disease_mean.shape)
print(data_disease_min.shape)
print(data_disease_max.shape)
```

```
(4802, 3)
(4802, 3)
(4802, 3)
(4802, 3)
```

[237]:

```
data_disease_summary = data_disease_median.merge(data_disease_mean,
                                                 left_on = ['std_name',␣
 ↪'symptom_name'],
                                                 right_on = ['std_name',␣
 ↪'symptom_name'],
                                                 how = "inner")

data_disease_summary = data_disease_summary.merge(data_disease_min,
                                                  left_on = ['std_name',␣
 ↪'symptom_name'],
                                                  right_on = ['std_name',␣
 ↪'symptom_name'],
                                                  how = "inner")

data_disease_summary = data_disease_summary.merge(data_disease_max,
                                                  left_on = ['std_name',␣
 ↪'symptom_name'],
                                                  right_on = ['std_name',␣
 ↪'symptom_name'],
                                                  how = "inner")

print(data_disease_summary.shape)
data_disease_summary.head()
```

```
(4802, 6)
```

[237]:

```
                     std_name symptom_name    median      mean       min  \
0  (-)-Deoxypodophyllotoxin   no symptom  0.517772  0.621357  0.328342
1          (-)-Gambogic Acid   no symptom  0.368344  0.480085 -0.008534
2          (-)-NORADRENALINE   meningioma  0.893658  0.884852  0.741394
3          (-)-NORADRENALINE   no symptom  1.038622  1.019079  0.384903
4          (-)-NORADRENALINE          pNF  1.017886  1.021358  0.616536

        max
0  1.284884
1  1.130643
2  1.023629
3  1.172962
4  1.238870
```

[238]:

```
## https://towardsdatascience.com/
 ↪name-your-favorite-excel-function-and-ill-teach-you-its-pandas-equivalent-7ee4400ada9f
data_disease_summary['disease_name'] = \
    data_disease_summary.symptom_name.map(df_cell_disease.
 ↪set_index('symptom_name')['disease_name'].to_dict())

data_disease_summary.head()
```

[238]:

```
                     std_name symptom_name    median      mean       min  \
0  (-)-Deoxypodophyllotoxin   no symptom  0.517772  0.621357  0.328342
1          (-)-Gambogic Acid   no symptom  0.368344  0.480085 -0.008534
2          (-)-NORADRENALINE   meningioma  0.893658  0.884852  0.741394
3          (-)-NORADRENALINE   no symptom  1.038622  1.019079  0.384903
4          (-)-NORADRENALINE          pNF  1.017886  1.021358  0.616536

        max disease_name
0  1.284884          NF2
1  1.130643          NF2
2  1.023629          NF2
3  1.172962          NF2
4  1.238870          NF1
```

[364]:

```
print(data_disease_summary.dtypes)
data_disease_summary['std_name'] = data_disease_summary.std_name.astype(str)
```

```
std_name         object
symptom_name     object
median          float64
mean            float64
min             float64
max             float64
disease_name     object
```

```
dtype: object
```

[239]:
```
# saved as csv file since takes some time to run
data_disease_summary.to_csv('../assets/data_disease_summary.csv', index=False)
```

2.3.3 Meningioma

[533]:
```
df_meningioma = data.copy()
df_meningioma = df_meningioma[(df_meningioma.symptom_name == 'meningioma')]
df_meningioma.shape
```

[533]:
```
(26288, 17)
```

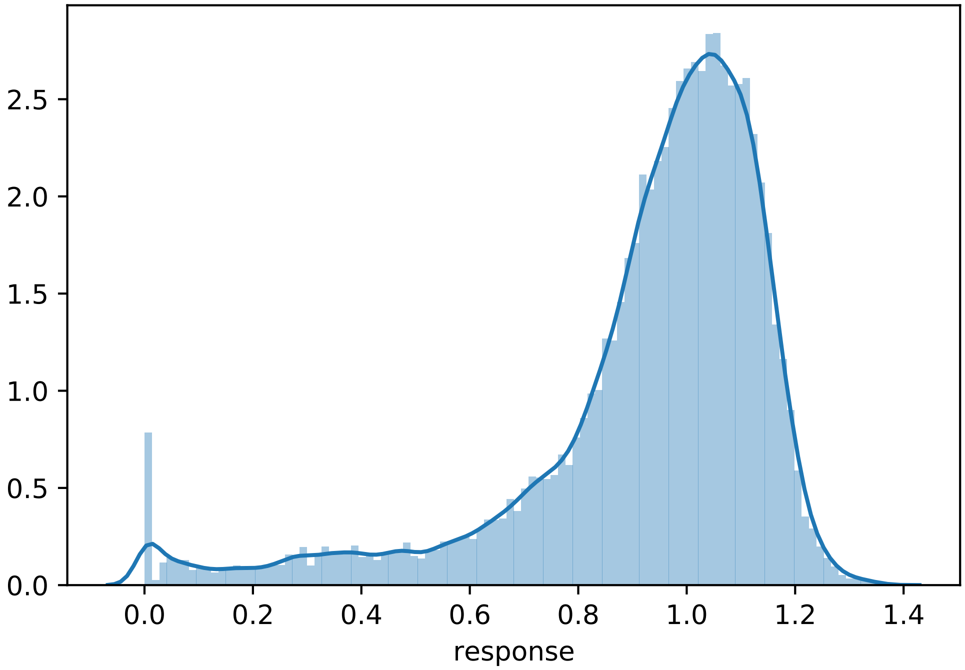
[534]:
```
df_meningioma.organism_name.value_counts()
```

[534]:
```
human    26288
Name: organism_name, dtype: int64
```

[535]:
```
df_meningioma.model_name.value_counts()
```

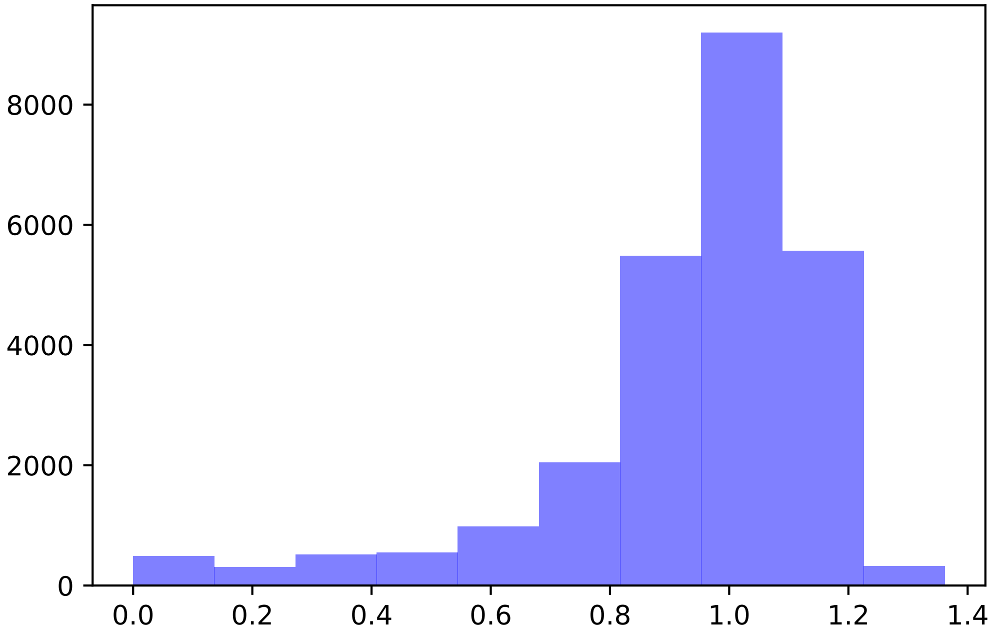
[535]:
```
Ben-Men-1    25448
Syn7           280
Syn10          280
Syn12          280
Name: model_name, dtype: int64
```

[536]:
```
sns.distplot(df_meningioma.response, bins = 100);
```



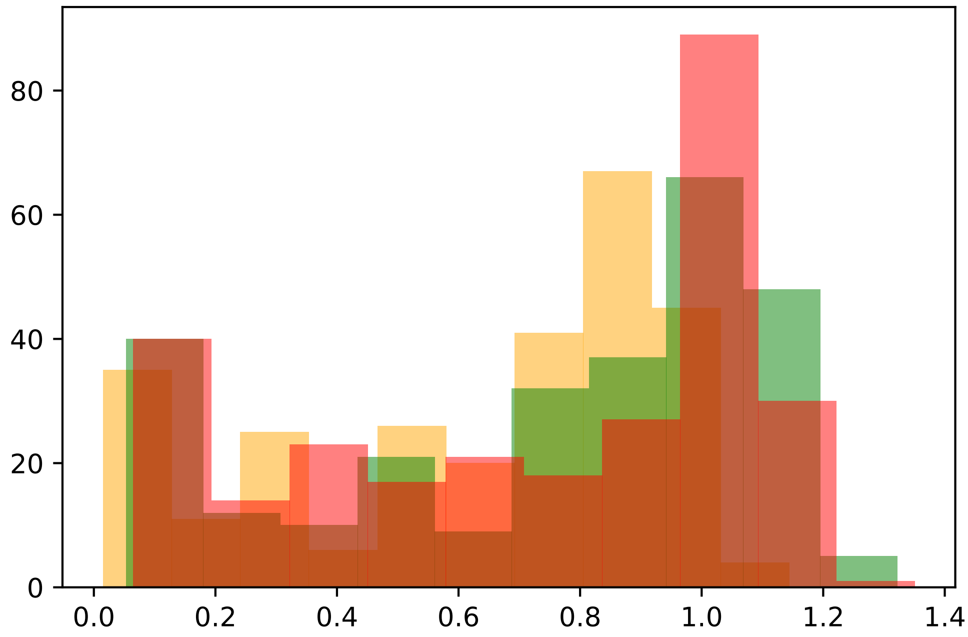
[537]:

```
plt.hist(df_meningioma.response[(df_meningioma.model_name == 'Ben-Men-1')],␣
 ↪alpha = 0.5, color = 'blue');
```



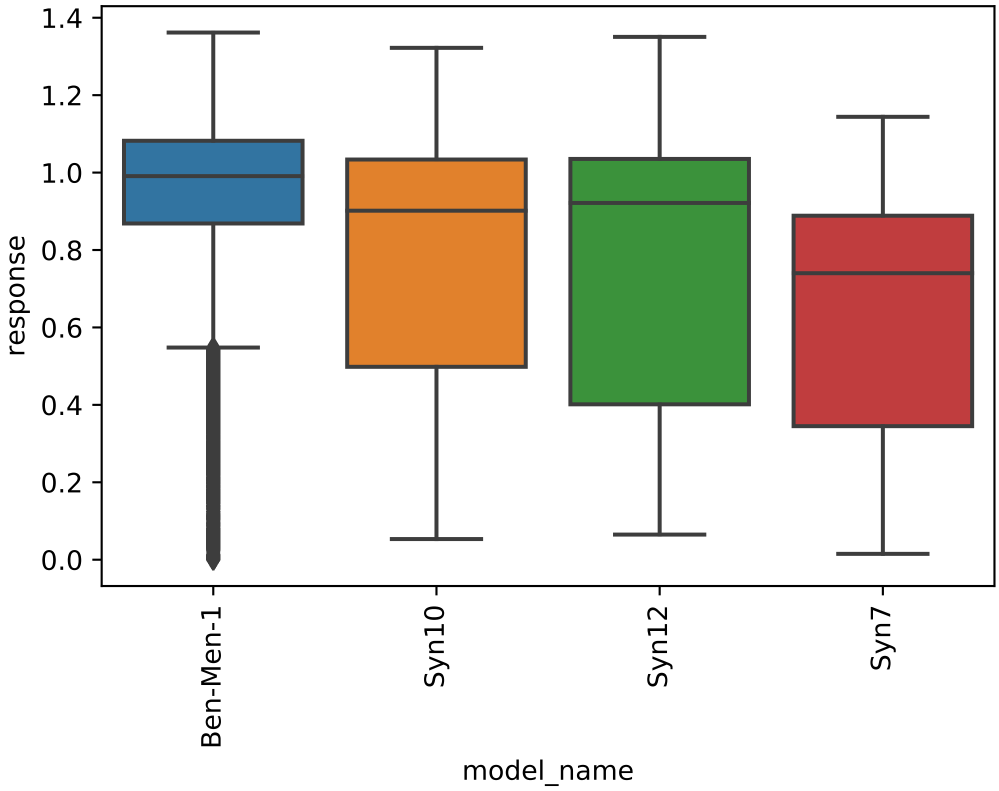
[538]:

```
plt.hist(df_meningioma.response[(df_meningioma.model_name == 'Syn7')], alpha =␣
 ↪0.5, color = 'orange');
plt.hist(df_meningioma.response[(df_meningioma.model_name == 'Syn10')], alpha =␣
 ↪0.5, color = 'green');
plt.hist(df_meningioma.response[(df_meningioma.model_name == 'Syn12')], alpha =␣
 ↪0.5, color = 'red');
```



Consider normalizing % viability output

```
[539]: ax = sns.boxplot(x = 'model_name', y = 'response', data = df_meningioma);
       ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);
```



2.3.4 Schwannoma

```
[540]: df_schwannoma = data.copy()
       df_schwannoma = df_schwannoma[(df_schwannoma.symptom_name == 'schwannoma')]
       df_schwannoma.shape
```

```
[540]: (22950, 17)
```

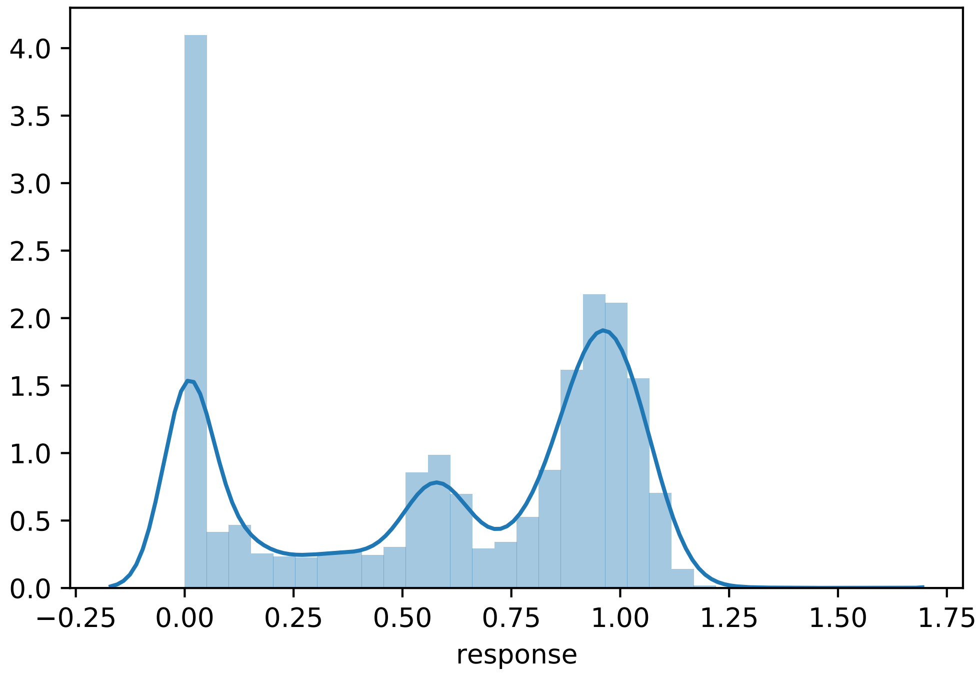
```
[541]: df_schwannoma.organism_name.value_counts()
```

```
[541]: mouse    22950
       Name: organism_name, dtype: int64
```

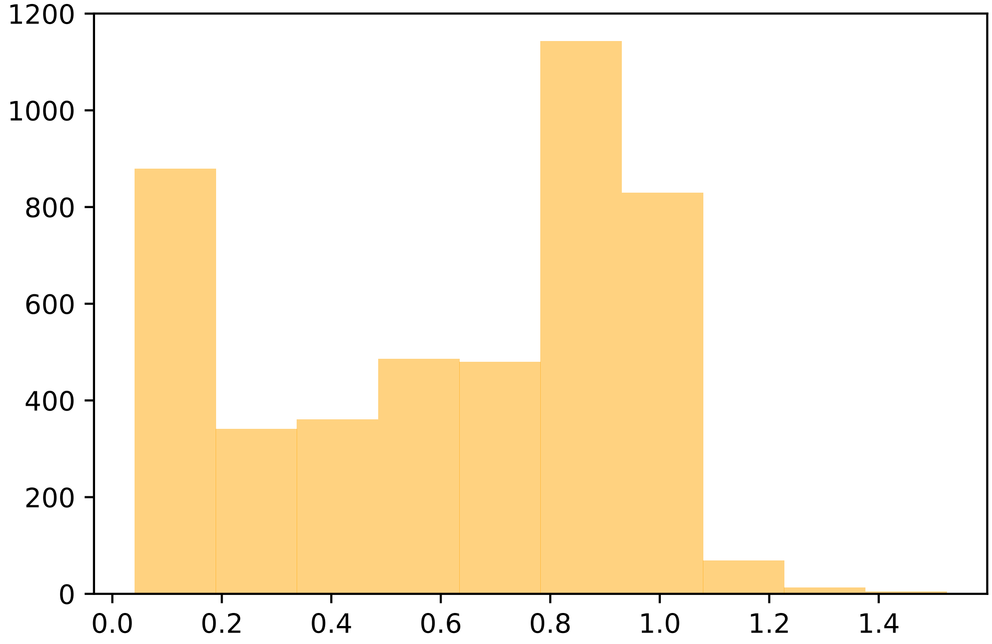
```
[542]: df_schwannoma.model_name.value_counts()
```

```
[542]: MS02    17192
       MS01     4606
       MS03     1152
       Name: model_name, dtype: int64
```

```
[543]: sns.distplot(df_schwannoma.response, bins = 30);
```

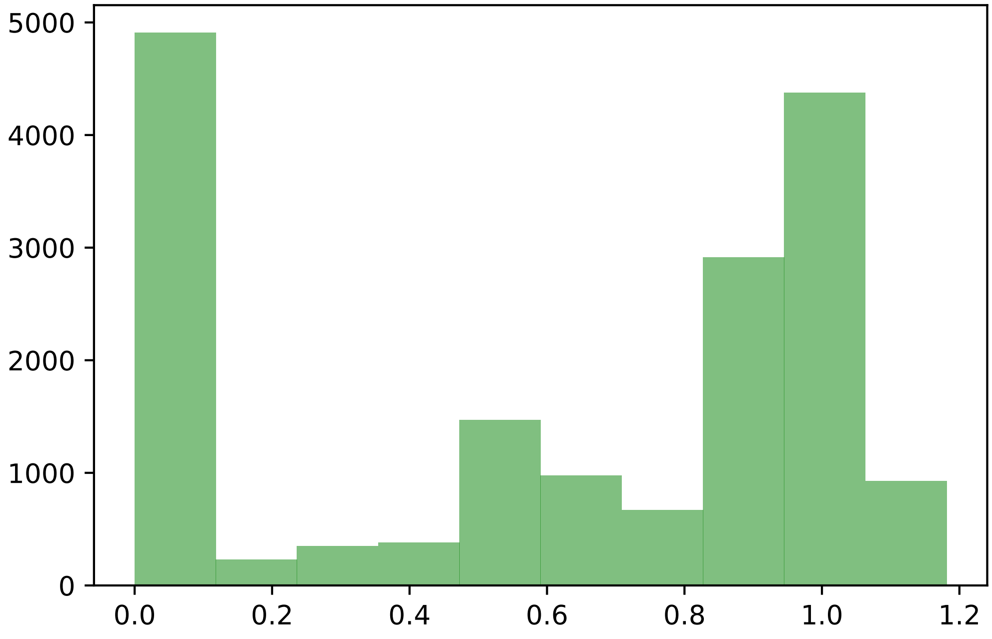


[544]:
```
plt.hist(df_schwannoma.response[(df_schwannoma.model_name == 'MS01')], alpha =␣
↪0.5, color = 'orange');
```



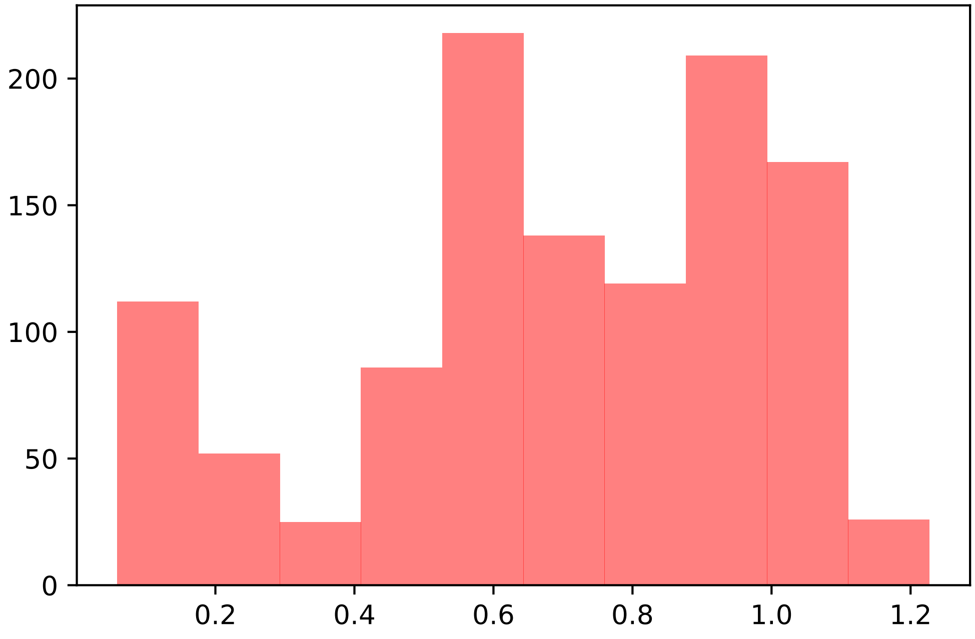
[545]:

```
plt.hist(df_schwannoma.response[(df_schwannoma.model_name == 'MS02')], alpha =␣
↪0.5, color = 'green');
```

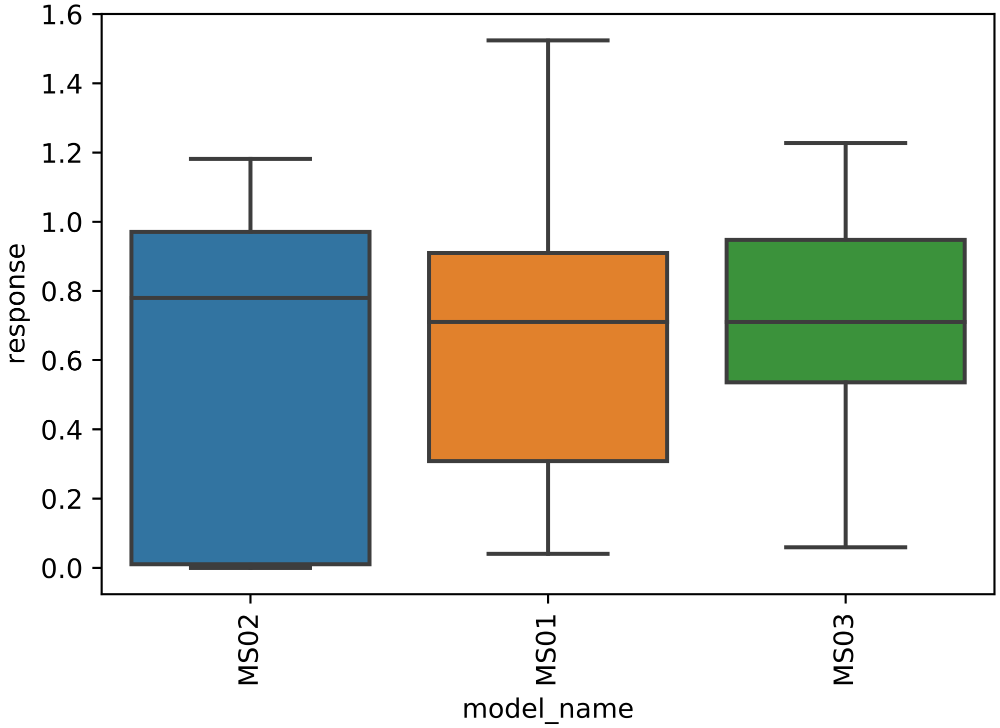


[546]:

```
plt.hist(df_schwannoma.response[(df_schwannoma.model_name == 'MS03')], alpha =␣
↪0.5, color = 'red');
```



[547]:
```
ax = sns.boxplot(x = 'model_name', y = 'response', data = df_schwannoma);
ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);
```



2.3.5 pNF

[548]:
```
df_plexiform = data.copy()
df_plexiform = df_plexiform[(df_plexiform.symptom_name == 'pNF')]
df_plexiform.shape
```

[548]:
```
(88088, 17)
```

[549]:
```
df_plexiform.organism_name.value_counts()
```

[549]:
```
human    88088
Name: organism_name, dtype: int64
```

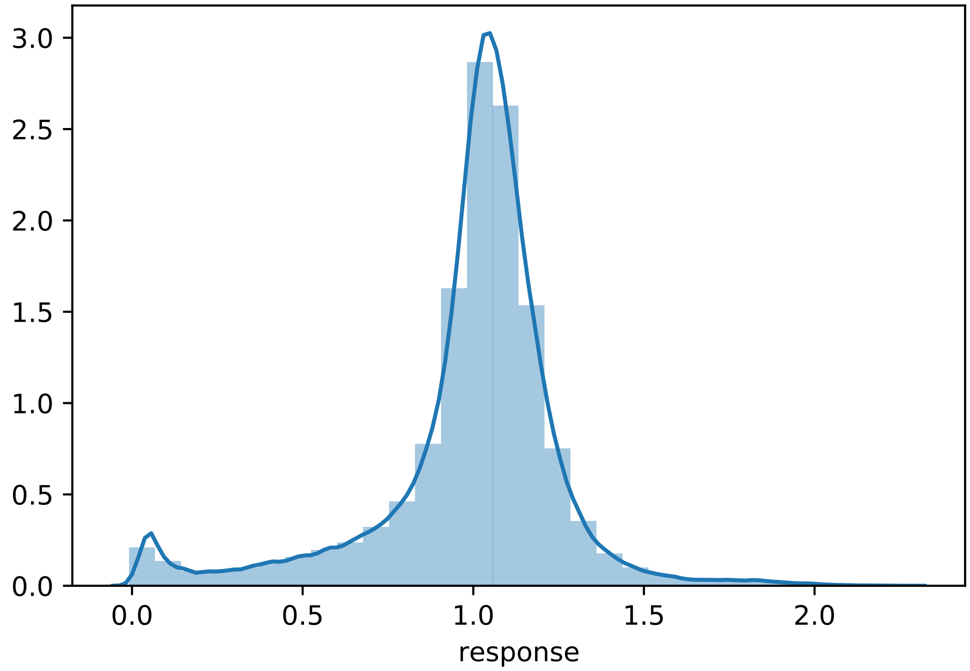
[550]:
```
df_plexiform.model_name.value_counts()
```

[550]:
```
ipNF95.6                    12584
ipNF95.11b C                12584
ipNF05.5 (single clone)     12584
```

```
ipNF05.5 (mixed clone)     12584
ipnNF95.11C                12584
ipNF06.2A                  12584
ipNF95.11b C/T             12584
Name: model_name, dtype: int64
```

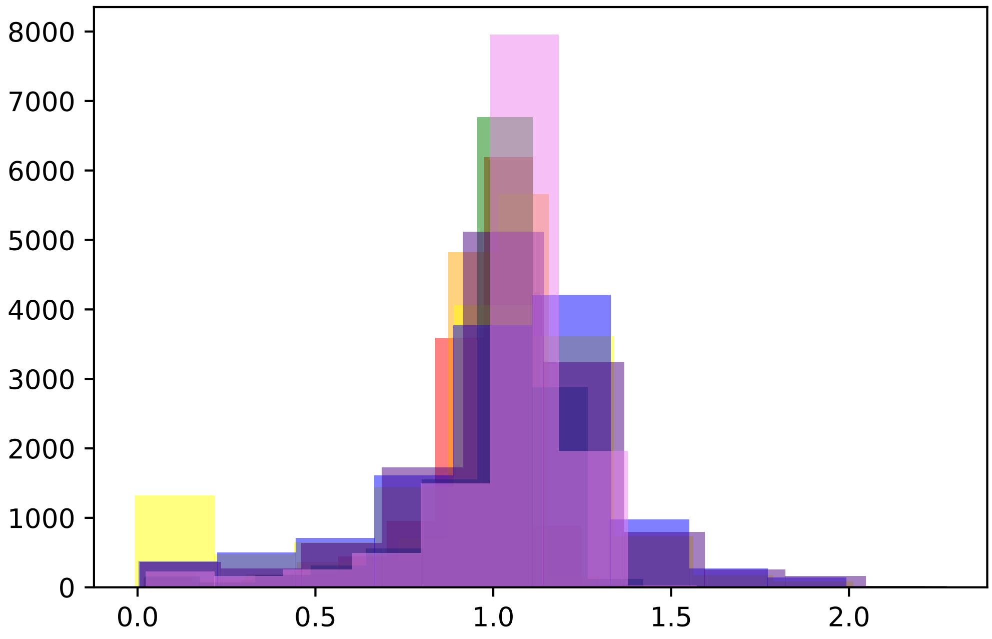
[551]:

```
sns.distplot(df_plexiform.response, bins = 30);
```

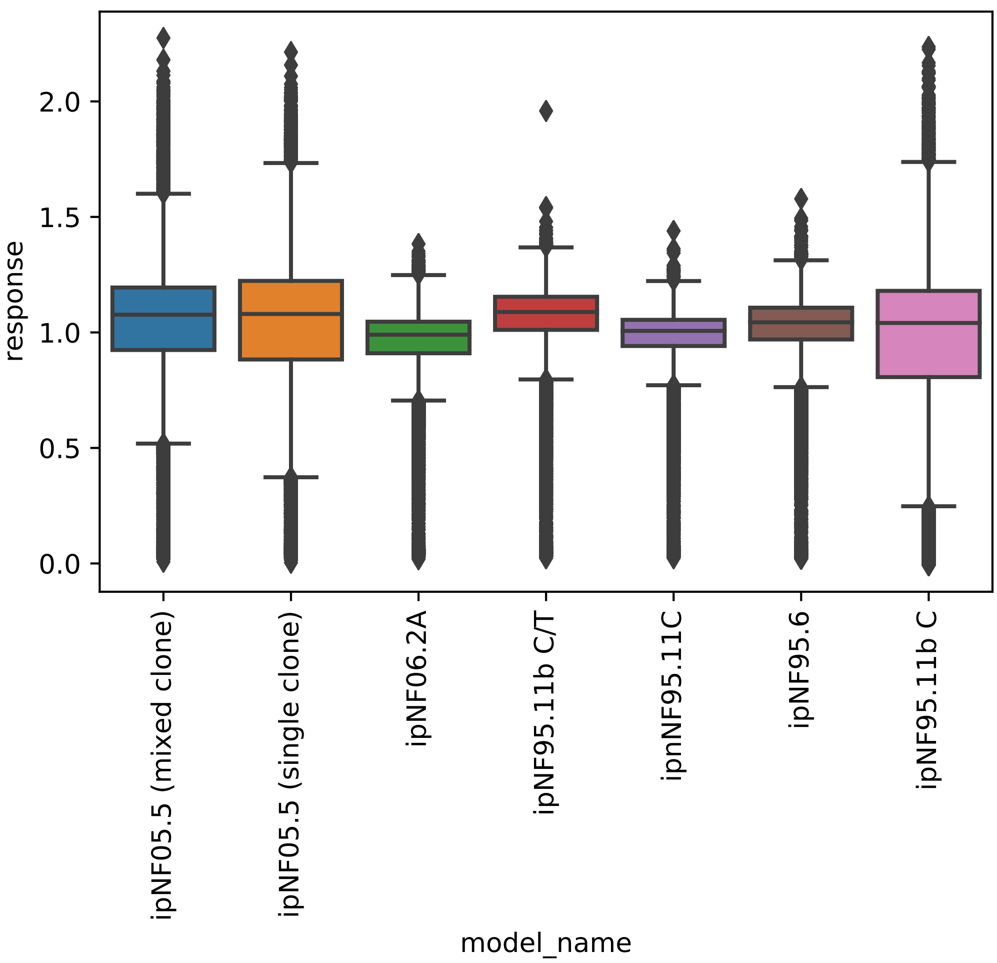


[552]:

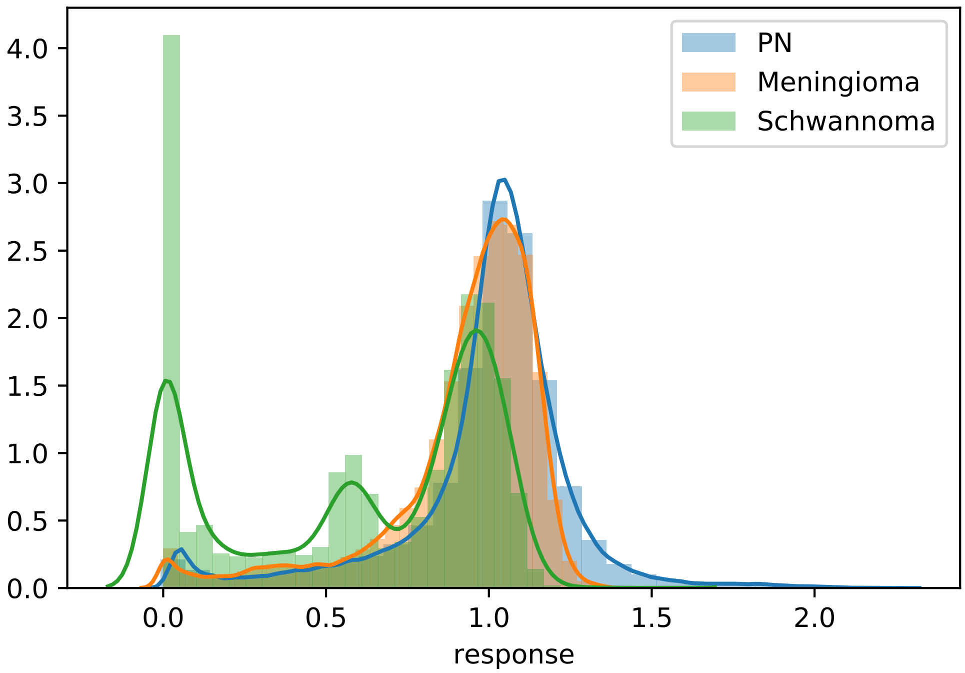
```
plt.hist(df_plexiform.response[(df_plexiform.model_name == 'ipNF06.2A')], alpha␣
 ↪= 0.5, color = 'red');
plt.hist(df_plexiform.response[(df_plexiform.model_name == 'ipnNF95.11C')],␣
 ↪alpha = 0.5, color = 'orange');
plt.hist(df_plexiform.response[(df_plexiform.model_name == 'ipNF95.11b C')],␣
 ↪alpha = 0.5, color = 'yellow');
plt.hist(df_plexiform.response[(df_plexiform.model_name == 'ipNF95.6')], alpha␣
 ↪= 0.5, color = 'green');
plt.hist(df_plexiform.response[(df_plexiform.model_name == 'ipNF05.5 (single␣
 ↪clone)')], alpha = 0.5, color = 'blue');
plt.hist(df_plexiform.response[(df_plexiform.model_name == 'ipNF05.5 (mixed␣
 ↪clone)')], alpha = 0.5, color = 'indigo');
plt.hist(df_plexiform.response[(df_plexiform.model_name == 'ipNF95.11b C/T')],␣
 ↪alpha = 0.5, color = 'violet');
```



```
[553]: ax = sns.boxplot(x = 'model_name', y = 'response', data = df_plexiform);
       ax = ax.set_xticklabels(ax.get_xticklabels(),rotation=90);
```



```
[554]: sns.distplot(df_plexiform.response, bins = 30);
       sns.distplot(df_meningioma.response, bins = 30);
       sns.distplot(df_schwannoma.response, bins = 30);
       plt.legend(['PN', 'Meningioma', 'Schwannoma']);
```



3 Prep Journal Articles

```
[61]: df_journal.meta_language.value_counts()
```

```
[61]: English       5164
      Spanish         94
      Japanese        90
      French          84
      Chinese         64
      German          59
      Russian         29
      Turkish         24
      Dutch           14
      Portuguese      13
      Czech           10
      Polish          10
      Korean          10
      Italian          8
      Hungarian        8
      Bulgarian        5
      Serbian          3
      Persian          2
      Croatian         2
      Swedish          2
```

```
Danish            2
Estonian          1
Romanian          1
Greek             1
Slovak            1
Arabic            1
Name: meta_language, dtype: int64
```

[62]:
```
df_journal.columns
```

[62]:
```
Index(['Eid', 'abstract', 'affiliation_organization', 'title', 'year',
       'sourcetitle', 'issn_print', 'doi', 'openaccess', 'meta_language',
       'References', 'pmid', 'publishername', 'keywords', 'funding_text'],
      dtype='object')
```

[63]:
```
df_journal_en = df_journal.copy()
df_journal_en = df_journal_en[(df_journal_en.meta_language == 'English')]
df_journal_en.reset_index(drop=True, inplace=True)
```

[64]:
```
df_journal_en.shape
```

[64]:
```
(5164, 15)
```

[65]:
```
df_journal_en['meningioma'] = list(df_journal_en.abstract.apply(lambda x: 1 if␣
 ↪str(x).lower().find('meningioma')>=0 else 0))

df_journal_en['schwannoma'] = list(df_journal_en.abstract.apply(lambda x: 1 if␣
 ↪str(x).lower().find('schwannoma')>=0 else 0))

df_journal_en['plexiform'] = list(df_journal_en.abstract.apply(lambda x: 1 if␣
 ↪str(x).lower().find('plexiform')>=0 else 0))
```

[66]:
```
abstract_series = df_journal_en.abstract.replace("-", "", regex = True).str.
 ↪lower()

abstract_series
```

[66]:
```
0       introduction. neurofibromatosis type 1 is an a…
1                                                   NaN
2       malignant peripheral nerve sheath tumors accou…
3       we report a 20yearold man with cauda equina sy…
4       objective:: to determine the best surgical str…
                              …
5159    neurofibromatosis type 1 (nf1) is a common tum…
5160    stereotactic radiosurgery (srs) has been used …
5161    purpose:to evaluate the natural history of mye…
5162    purpose: although some specific genetic syndro…
```

```
5163    vasculopathy is a wellrecognized abnormality a…
Name: abstract, Length: 5164, dtype: object
```

3.1 Drugs from Target Explorer

3.1.1 Meningioma

[172]:

```
abstract_meningioma = abstract_series[(df_journal_en.meningioma == 1)]
abstract_no_list = abstract_meningioma.index.to_list()
abstract_meningioma.reset_index(drop=True, inplace=True)
abstract_meningioma = pd.DataFrame({'abstract': abstract_meningioma,
                                   'abstract_no': abstract_no_list})
```

[173]:

```
drugs_meningioma = data_disease_summary.std_name.loc[(data_disease_summary.
 ↪symptom_name == 'meningioma')]

## replace - with ""
drugs_meningioma = drugs_meningioma.replace("-", "", regex = True)
## set all values lower case
drugs_meningioma = drugs_meningioma.str.lower()
## remove white spaces
# drugs_meningioma = drugs_meningioma.str.strip()
## remove duplicates
drugs_meningioma = list(set(drugs_meningioma.to_list()))

print(len(drugs_meningioma))
```

```
1144
```

[174]:

```
idx_list_meningioma = []

for n in drugs_meningioma:
    temp_list = abstract_meningioma.abstract.str.find(n).to_list()
    temp_idx = [i for i, j in enumerate(temp_list) if j >= 0]
    idx_list_meningioma.append(temp_idx)

idx_drug_meningioma = [i for i, j in enumerate(idx_list_meningioma) if j != []]
drug_list_meningioma = [drugs_meningioma[i] for i in idx_drug_meningioma]
idx_list_meningioma = [i for i in idx_list_meningioma if i != []]
```

[175]:

```
print(idx_list_meningioma)
print()
print(drug_list_meningioma)
```

```
[[77], [207], [30, 87], [24], [49], [49], [109], [33], [46, 51, 107, 122, 139],
[234], [53, 207], [30], [114], [33], [38, 87, 144], [0, 87], [0], [38, 49, 87],
[30], [30], [83], [226], [0], [66], [30], [49, 87], [24], [234], [30]]
```

```
['torin1', 'ar12', 'erlotinib', 'panobinostat', 'nilotinib', 'selumetinib',
'levetiracetam', 'doxorubicin', 'progesterone', 'lovastatin', 'ar42',
'verapamil', 'dasatinib', 'etoposide', 'apatinib', 'everolimus', 'temsirolimus',
'sorafenib', 'hydroxyurea', 'tamoxifen', 'cytidine', 'azd2014', 'uridine',
'crizotinib', 'metformin', 'imatinib', 'cudc907', 'vincristine', 'mifepristone']
```

[176]:

```
df_meningioma = abstract_meningioma.loc[[item for sublist in␣
 ↪idx_list_meningioma for item in sublist], :]
df_meningioma.reset_index(drop=True, inplace =True)

len_list = [len(i) for i in idx_list_meningioma]
drug_list_rep = np.repeat(drug_list_meningioma, len_list, axis=0)
df_meningioma['drug'] = drug_list_rep

df_meningioma['condition'] = 'meningioma'

print(df_meningioma.shape)
df_meningioma.head()
```

```
(41, 4)
```

[176]:

```
                                            abstract  abstract_no  \
0  inactivating mutations in the neurofibromatosi…         1406
1  meningiomas constitute about 34% of primary in…         4003
2  purpose: the purpose was to reevaluate in cell…          542
3  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549
4  neurofibromatosis 2 (nf2) is a rare tumor supp…          355

           drug   condition
0        torin1  meningioma
1          ar12  meningioma
2     erlotinib  meningioma
3     erlotinib  meningioma
4  panobinostat  meningioma
```

[182]:

```
df_meningioma[(df_meningioma.drug == 'mifepristone')]
```

[182]:

```
                                             abstract  abstract_no  \
40  purpose: the purpose was to reevaluate in cell…          542

            drug   condition
40  mifepristone  meningioma
```

Encouraging - text near mifepristone negative and limited apparent activity in meningioma cell lines on average/median

[183]:

```
df_meningioma.abstract[40]
```

[183]:

```
'purpose: the purpose was to reevaluate in cell culture models the therapeutic
usefulness of some discussed chemotherapies or targeted therapies for
meningiomas with a special emphasis on the role of the neurofibromatosis type 2
(nf2) tumor suppressor, which had been neglected so far. in addition, the study
intended to evaluate a potential benefit from a treatment with drugs which are
well established in other fields of medicine and have been linked recently with
tumor disease by epidemiological studies. methods: meningioma cell lines
corresponding to various subtypes and pairs of syngenic meningioma cell lines
with or without shrnainduced nf2 knockdown were analyzed for their dosedependent
response to the drugs in microtiter tetrazolium assays, brdu assays and for
selected cases in elisas measuring nucleosome liberation to specifically
separate cell death from pure inhibition of cell proliferation. results: we
confirmed a moderate efficacy of hydroxyurea (hu) in clinically relevant
concentrations. under appropriate dosing, we neither detected major responses to
the alkylating compound temozolomide nor to various drugs targeting membrane
receptors or enzymes (tamoxifen, erlotinib, mifepristone, losartan, metformin
and verapamil). only concentrations far beyond achievable serum levels generated
significant effects with the exception of losartan, which showed no effects at
all. chemosensitivity varied markedly among meningioma cell lines. importantly,
cells with nf2 loss exhibited a significantly higher induction of cell death by
hu. conclusions: alternative chemotherapeutic or targeted approaches besides hu
have still to be evaluated in further studies, and the role of nf2 must be taken
into account. © 2014 springerverlag.'
```

[180]:

```
data_disease_summary.loc[(data_disease_summary.std_name.str.lower() ==␣
↪'torin1')]
```

[180]:

```
     std_name symptom_name    median      mean       min       max  \
4499   torin1   meningioma  0.580944  0.605717  0.303217  0.973232
4500   torin1   no symptom  0.728849  0.717262  0.309821  1.186820
4501   torin1          pNF  0.666697  0.694005  0.051281  1.190474
4502   torin1   schwannoma  0.486257  0.466251  0.289369  0.633625

     disease_name
4499          NF2
4500          NF2
4501          NF1
4502          NF2
```

3.1.2 Schwannoma

[184]:

```
abstract_schwannoma = abstract_series[(df_journal_en.schwannoma == 1)]
abstract_no_list = abstract_schwannoma.index.to_list()
abstract_schwannoma.reset_index(drop=True, inplace=True)
abstract_schwannoma = pd.DataFrame({'abstract': abstract_schwannoma,
                                    'abstract_no': abstract_no_list})
```

[185]:
```
drugs_schwannoma = data_disease_summary.std_name.loc[(data_disease_summary.
 ↪symptom_name == 'schwannoma')]

## replace - with ""
drugs_schwannoma = drugs_schwannoma.replace("-", "", regex = True)
## set all values lower case
drugs_schwannoma = drugs_schwannoma.str.lower()
## remove white spaces
# drugs_schwannoma = drugs_schwannoma.str.strip()
## remove duplicates
drugs_schwannoma = list(set(drugs_schwannoma.to_list()))

print(len(drugs_schwannoma))
```

```
1146
```

[186]:
```
idx_list_schwannoma = []

for n in drugs_schwannoma:
    temp_list = abstract_schwannoma.abstract.str.find(n).to_list()
    temp_idx = [i for i, j in enumerate(temp_list) if j >= 0]
    idx_list_schwannoma.append(temp_idx)

idx_drug_schwannoma = [i for i, j in enumerate(idx_list_schwannoma) if j != []]
drug_list_schwannoma = [drugs_schwannoma[i] for i in idx_drug_schwannoma]
idx_list_schwannoma = [i for i in idx_list_schwannoma if i != []]
```

[187]:
```
print(idx_list_schwannoma)
print()
print(drug_list_schwannoma)
```

```
[[416], [215], [204, 237, 356, 547, 561], [65], [212], [58], [129, 478], [129],
[571], [254], [90], [629], [665], [254], [254], [136, 413], [100, 237, 263, 348,
356, 394, 411, 478, 561], [16, 234], [212], [90], [100, 237, 263, 348, 356, 394,
411, 478, 561], [4, 221, 237, 356, 395, 478, 561], [672], [100, 129, 237],
[680], [123], [641], [347], [192, 234, 421], [529, 561], [17, 129, 237, 662],
[58], [212], [665]]

['vandetanib', 'torin1', 'erlotinib', 'lenalidomide', 'saracatinib',
'panobinostat', 'nilotinib', 'selumetinib', 'curcumin', 'cobimetinib',
'doxorubicin', 'dutasteride', 'lovastatin', 'trametinib', 'pd0325901', 'ar42',
'lapatinib', 'morin', 'dasatinib', 'etoposide', 'apatinib', 'everolimus',
'necrostatin', 'sorafenib', 'hydrocortisone', 'tamoxifen', 'ponatinib',
'uridine', 'crizotinib', 'aspirin', 'imatinib', 'cudc907', 'cabozantinib',
'vincristine']
```

[188]:

```
df_schwannoma = abstract_schwannoma.loc[[item for sublist in␣
 ↪idx_list_schwannoma for item in sublist], :]
df_schwannoma.reset_index(drop=True, inplace =True)

len_list = [len(i) for i in idx_list_schwannoma]
drug_list_rep = np.repeat(drug_list_schwannoma, len_list, axis=0)
df_schwannoma['drug'] = drug_list_rep

df_schwannoma['condition'] = 'schwannoma'

print(df_schwannoma.shape)
df_schwannoma.head()
```

```
(71, 4)
```

[188]:

```
                                            abstract  abstract_no        drug  \
0  patients with bilateral vestibular schwannomas…         2886  vandetanib
1  inactivating mutations in the neurofibromatosi…         1406      torin1
2  objectives: vestibular schwannomas are the hal…         1333   erlotinib
3  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549   erlotinib
4  the understanding of the molecular pathways un…         2421   erlotinib

    condition
0  schwannoma
1  schwannoma
2  schwannoma
3  schwannoma
4  schwannoma
```

[189]:

```
df_schwannoma[(df_schwannoma.drug == 'lapatinib')]
```

[189]:

```
                                             abstract  abstract_no       drug  \
22  loss of the tumor suppressor merlin causes dev…          683  lapatinib
23  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549  lapatinib
24  this singleinstitution phase ii study was perf…         1771  lapatinib
25  background: pharmacologic agents targeted agai…         2380  lapatinib
26  the understanding of the molecular pathways un…         2421  lapatinib
27  vestibular schwannomas (vs) arising sporadical…         2696  lapatinib
28  introduction: epidermal growth factor receptor…         2843  lapatinib
29  neurofibromatosis type 2 (nf2), a neurogenetic…         3318  lapatinib
30  medical therapy target population adults with …         3792  lapatinib

     condition
22  schwannoma
23  schwannoma
24  schwannoma
25  schwannoma
```

```
26   schwannoma
27   schwannoma
28   schwannoma
29   schwannoma
30   schwannoma
```

Encouraging - the median lapatinib effect in schwannoma cell line is fairly low and the language around lapatinib in abstract is fairly positive

[190]:
```
df_schwannoma.abstract[22]
```

[190]:
```
'loss of the tumor suppressor merlin causes development of the tumors of the
nervous system, such as schwannomas, meningiomas, and ependymomas occurring
spontaneously or as part of a hereditary disease neurofibromatosis type 2 (nf2).
current therapies, (radio) surgery, are not always effective. therefore, there
is a need for drug treatments for these tumors. schwannomas are the most
frequent of merlindeficient tumors and are hallmark for nf2. using our in vitro
human schwannoma model, we demonstrated that merlindeficiency leads to increased
proliferation, cellmatrix adhesion, and survival. increased proliferation due to
strong activation of extracellularsignalregulated kinase 1/2 (erk1/2) is caused
by overexpression/activation of plateletderived growth factor receptor  (pdgfr )
and erbb2/3 which we successfully blocked with azd6244, sorafenib, or lapatinib.
schwannoma basal proliferation is, however, only partly dependent on pdgfr  and
is completely independent of erbb2/3. moreover, the mechanisms underlying
pathological cellmatrix adhesion and survival of schwannoma cells are still not
fully understood. here, we demonstrate that insulinlike growth factori receptor
(igfir) is strongly overexpressed and activated in human primary schwannoma
cells. igfi and ii are overexpressed and released from schwannoma cells. we show
that erk1/2 is relevant for igfimediated increase in proliferation and
cellmatrix adhesion, cjun nterminal kinases for increased proliferation and akt
for survival. we demonstrate new mechanisms involved in increased basal
proliferation, cellmatrix adhesion, and survival of schwannoma cells. we
identified therapeutic targets igfir and downstream pi3k for treatment of
schwannoma and other merlindeficient tumors and show usefulness of small
molecule inhibitors in our model. pi3k is relevant for both igfir and previously
described pdgfr  signaling in schwannoma. © 2012 wiley periodicals, inc.'
```

[83]:
```
data_disease_summary.loc[(data_disease_summary.std_name.str.lower() ==␣
 ↪'lapatinib')]
```

[83]:
```
        std_name symptom_name    median      mean       min       max  \
2817   lapatinib   no symptom  0.855447  0.677948  0.004138  1.572811
2818   lapatinib   schwannoma  0.299060  0.438209  0.001851  1.304557

     disease_name
2817          NF2
2818          NF2
```

3.1.3 pNF

[191]:

```
abstract_plexiform = abstract_series[(df_journal_en.plexiform == 1)]
abstract_no_list = abstract_plexiform.index.to_list()
abstract_plexiform.reset_index(drop=True, inplace=True)
abstract_plexiform = pd.DataFrame({'abstract': abstract_plexiform,
                                   'abstract_no': abstract_no_list})
```

[192]:

```
drugs_plexiform = data_disease_summary.std_name.loc[(data_disease_summary.
 ↪symptom_name == 'pNF')]

## replace - with ""
drugs_plexiform = drugs_plexiform.replace("-", "", regex = True)
## set all values lower case
drugs_plexiform = drugs_plexiform.str.lower()
## remove white spaces
# drugs_plexiform = drugs_plexiform.str.strip()
## remove duplicates
drugs_plexiform = list(set(drugs_plexiform.to_list()))

print(len(drugs_plexiform))
```

```
1142
```

[193]:

```
idx_list_plexiform = []

for n in drugs_plexiform:
    temp_list = abstract_plexiform.abstract.str.find(n).to_list()
    temp_idx = [i for i, j in enumerate(temp_list) if j >= 0]
    idx_list_plexiform.append(temp_idx)

idx_drug_plexiform = [i for i, j in enumerate(idx_list_plexiform) if j != []]
drug_list_plexiform = [drugs_plexiform[i] for i in idx_drug_plexiform]
idx_list_plexiform = [i for i in idx_list_plexiform if i != []]
```

[194]:

```
print(idx_list_plexiform)
print()
print(drug_list_plexiform)
```

```
[[101, 107, 264], [343], [228, 315, 366], [345], [50, 118], [143, 220, 351],
[311, 353], [39, 42, 146], [27, 101, 107], [335], [75, 220], [45, 127, 330],
[23], [264], [345], [106], [264], [45], [345], [107], [42], [343], [325], [33,
50, 148, 266, 340], [33], [330], [335]]

['estradiol', 'mycophenolate mofetil', 'tipifarnib', 'tetracycline',
'nilotinib', 'selumetinib', 'curcumin', 'doxorubicin', 'progesterone',
'lovastatin', 'trametinib', 'pd0325901', 'ketotifen', 'trifluoperazine',
'doxycycline', 'sorafenib', 'tamoxifen', 'azd8055', 'minocycline',
'testosterone', 'pd98059', 'tacrolimus', 'sunitinib', 'imatinib', 'octreotide',
'ly294002', 'vincristine']
```

[195]:

```
df_plexiform = abstract_plexiform.loc[[item for sublist in idx_list_plexiform␣
 ↪for item in sublist], :]
df_plexiform.reset_index(drop=True, inplace =True)

len_list = [len(i) for i in idx_list_plexiform]
drug_list_rep = np.repeat(drug_list_plexiform, len_list, axis=0)
df_plexiform['drug'] = drug_list_rep

df_plexiform['condition'] = 'pNF'

print(df_plexiform.shape)
df_plexiform.head()
```

```
(46, 4)
```

[195]:

```
                                            abstract  abstract_no  \
0  background:both the number and size of tumours…         1232
1  objective to assess the relationship between p…         1361
2  few therapeutic options are available for mali…         3454
3  background: on january 26, 2010, our team perf…         4714
4  backgroundras is dysregulated in neurofibromat…         2928

                  drug condition
0            estradiol       pNF
1            estradiol       pNF
2            estradiol       pNF
3  mycophenolate mofetil       pNF
4           tipifarnib       pNF
```

[196]:

```
data_cell_summary.loc[(data_cell_summary.std_name.str.lower() == 'selumetinib')]
```

[196]:

```
          std_name              model_name    median      mean       min  \
16441  SELUMETINIB                Ben-Men-1  1.000560  0.981389  0.644322
16442  SELUMETINIB                      HFF  1.111205  1.086076  0.960335
16443  SELUMETINIB                     HS01  0.009488  0.145295  0.006853
16444  SELUMETINIB                     MS01  0.787316  0.804071  0.410623
16445  SELUMETINIB                     MS02  0.007404  0.038811  0.001855
16446  SELUMETINIB                     MS03  0.744430  0.756368  0.425061
16447  SELUMETINIB                     MS11  0.897782  0.869672  0.475614
16448  SELUMETINIB                     MS12  0.898919  0.898168  0.555736
16449  SELUMETINIB                      MTC  1.051009  0.990937  0.575425
16450  SELUMETINIB                     Syn1  1.165672  1.123717  0.850596
16451  SELUMETINIB                     Syn5  1.070416  0.993586  0.520657
16452  SELUMETINIB   ipNF05.5 (mixed clone)  1.391732  1.256896  0.728744
```

```
16453  SELUMETINIB  ipNF05.5 (single clone)  1.301748  1.227528  0.788596
16454  SELUMETINIB                ipNF06.2A  1.000919  0.945547  0.677123
16455  SELUMETINIB             ipNF95.11b C  1.266695  1.162255  0.512811
16456  SELUMETINIB           ipNF95.11b C/T  1.066852  1.064258  0.920228
16457  SELUMETINIB                 ipNF95.6  1.114097  1.061559  0.697050
16458  SELUMETINIB                  ipn02.3  1.108281  1.087995  0.859000
16459  SELUMETINIB                  ipn02.8  1.025159  1.002086  0.775920
16460  SELUMETINIB              ipnNF95.11C  1.119192  1.086816  0.794945

            max
16441  1.207068
16442  1.214105
16443  1.278379
16444  1.072320
16445  1.056445
16446  1.062936
16447  1.146098
16448  1.270401
16449  1.193251
16450  1.271611
16451  1.194069
16452  1.496335
16453  1.399700
16454  1.118034
16455  1.513138
16456  1.158309
16457  1.194517
16458  1.174175
16459  1.171184
16460  1.213288
```

3.1.4 Combine all dataframes

[197]:
```
df_combined = pd.concat([df_meningioma, df_schwannoma, df_plexiform])
df_combined.reset_index(drop=True, inplace=True)
df_combined.head()
```

[197]:
```
                                            abstract  abstract_no  \
0  inactivating mutations in the neurofibromatosi…         1406
1  meningiomas constitute about 34% of primary in…         4003
2  purpose: the purpose was to reevaluate in cell…          542
3  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549
4  neurofibromatosis 2 (nf2) is a rare tumor supp…          355

          drug   condition
0       torin1  meningioma
1         ar12  meningioma
```

```
2     erlotinib  meningioma
3     erlotinib  meningioma
4  panobinostat  meningioma
```

[198]:
```
# saved as csv file since takes some time to run
df_combined.to_csv('../assets/abstracts_sorted.csv', index=False)
```

4 Pre-Process Abstracts

[3]:
```
disease_summary = pd.read_csv('../assets/data_disease_summary.csv', header=0)
abstracts = pd.read_csv('../assets/abstracts_sorted.csv', header=0)
```

[4]:
```
## standardize column names across the dataframe

# abstracts = abstracts.rename(columns={"drug": "std_name", "condition":␣
 ↪"symptom_name"})
disease_summary = disease_summary.rename(columns={"std_name": "drug",␣
 ↪"symptom_name": "condition"})

# df_combo = disease_summary.merge(abstracts, how = 'right', on =␣
 ↪['drug','condition'])
```

[5]:
```
## standardize drug names from disease_summary dataframe
## replace - with ""
disease_summary.drug = disease_summary.drug.replace("-", "", regex = True)
## set all values lower case
disease_summary.drug = disease_summary.drug.str.lower()
## remove white spaces
# disease_summary.drug = disease_summary.drug.str.strip()
```

[6]:
```
## all the apatinib rows actually just contain 'lopatinib' so dropped
abstracts = abstracts[abstracts.drug != 'apatinib']
## the 'morin' results from tumor-induced with - removed
abstracts = abstracts[abstracts.drug != 'morin']
abstracts.reset_index(drop=True, inplace=True)
```

[7]:
```
df_moa = pd.read_csv('../assets/moa.csv', header=0)
```

[8]:
```
## replace - with ""
df_moa.Drugs = df_moa.Drugs.replace("-", "", regex = True)
## set all values lower case
df_moa.Drugs = df_moa.Drugs.str.lower()

# df_moa = df_moa.drop_duplicates()
```

4.1 Normalize abstract text

[9]:

```
#Substitute Contractions
abstracts['abstract_norm'] = abstracts['abstract'].apply(lambda x:␣
 ↪[contractions.fix(word) for word in x.split()])
abstracts['abstract_norm'] = [' '.join(map(str, l)) for l in␣
 ↪abstracts['abstract_norm']]
#df_train['text_cf_numbers'] = df_train['text_contractions_fixed'].apply(lambda␣
 ↪x: [w2n.word_to_num(word) for word in x.split()])
abstracts.head(3)
```

[9]:

```
                                            abstract  abstract_no       drug  \
0  inactivating mutations in the neurofibromatosi…         1406     torin1
1  meningiomas constitute about 34% of primary in…         4003       ar12
2  purpose: the purpose was to reevaluate in cell…          542  erlotinib

    condition                                      abstract_norm
0  meningioma  inactivating mutations in the neurofibromatosi…
1  meningioma  meningiomas constitute about 34% of primary in…
2  meningioma  purpose: the purpose was to reevaluate in cell…
```

[10]:

```
#A function to clean the text
def normalize(text):
    text = remove_url(text)
    text = remove_html(text)
    text = normalize_foreign_char(text)
#     text = remove_numbers(text)
    text = remove_punctuation(text)
    #text = remove_whitespace(text)
    text = text.lower()
    return text

#Helper Functions
def remove_url(text):
    url = re.compile(r'https?://\S+|www\.\S+') #URLs
    text = url.sub(r'', text) #remove URLs
    return text

def remove_html(text):
    html=re.compile(r'<.*?>')
    text = html.sub(r'',text)
    return text

def remove_punctuation(text):
    table = str.maketrans('', '', string.punctuation)
    text = text.translate(table)
    return text
```

```
## this was removing numbers from drug names
def remove_numbers(text):
    text = ''.join(c for c in text if not c.isdigit())
    return text

def remove_whitespace(text):
    corrected = str(text)
    corrected = re.sub(r"//t",r"\t", corrected)
    corrected = re.sub(r"( )\1+",r"\1", corrected)
    corrected = re.sub(r"(\n)\1+",r"\1", corrected)
    corrected = re.sub(r"(\r)\1+",r"\1", corrected)
    corrected = re.sub(r"(\t)\1+",r"\1", corrected)
    return corrected.strip(" ")

def normalize_foreign_char(text):
    text = unidecode.unidecode(text)
    return text
```

[11]:
```
abstracts['abstract_norm'] = abstracts['abstract_norm'].apply(lambda x :␣
 ↪normalize(x))
abstracts.head(3)
```

[11]:
```
                                            abstract  abstract_no       drug  \
0  inactivating mutations in the neurofibromatosi…         1406     torin1
1  meningiomas constitute about 34% of primary in…         4003       ar12
2  purpose: the purpose was to reevaluate in cell…          542  erlotinib

    condition                                      abstract_norm
0  meningioma  inactivating mutations in the neurofibromatosi…
1  meningioma  meningiomas constitute about 34 of primary int…
2  meningioma  purpose the purpose was to reevaluate in cell …
```

4.2 Remove stopwords

[12]:
```
stop_words = set(stopwords.words('english'))

## add words/phrases to stop words
manual_sw = ['neurofibromatosis type', 'neurofibromatosis',
             'nf', 'nf1', 'nf2',
             'schwannomas', 'schwannoma',
             'meningioma', 'meningiomas',
             'ependymoma', 'ependymomas',
             'plexiform neurofibroma', 'plexiform neurofibroma',
             'plexiform', 'neurofibroma', 'neurofibromas',
             'pNF', 'pNFs', 'cell']
stop_words.update(manual_sw)
```

```
## add drugs to stopwords
df_drugs_list = abstracts.drug
drug_sw = list(df_drugs_list)
stop_words.update(df_drugs_list)

## stopwords now removed indirectly via 'context' columns
## no longer in use but preserved in case change order
# abstracts['stopwords_removed'] = abstracts['tokenized'].apply(lambda x: [word␣
 ↪for word in x if word not in stop_words])
# abstracts.head(3)
```

4.3 Extract +/-10 words from drug reference

[13]:

```
def remove_values_from_list(the_list, val):
    return [value for value in the_list if value != val]

#ten words before and after
def context(word, text, n=10):
    ## remove the drug's own name from stopwords
    sw_temp = stop_words.copy()
    sw_temp.remove(word)

    ## split abstract by spaces and remove stop words
    text = text.split()
    text = [i for i in text if i not in sw_temp]

    ## find locations where word occurs and extract n words before and after
    res = [i for i, j in enumerate(text) if word.split()[0] in j]
    new_text = []
    for j in res:
        new_text += text[j-n:j+(n+1)]
    unique_words = new_text
    unique_words = remove_values_from_list(unique_words, word)

    return unique_words
```

[14]:

```
#visual inspection change *ASSUMED true for all
#abstracts['drug'] = abstracts['drug'].apply(lambda x: x.replace('apatinib',␣
 ↪'lapatinib'))

#take 10+/- words
abstracts['context'] = abstracts.apply(lambda x: context(word = x['drug'], text␣
 ↪= x['abstract_norm']), axis=1)
abstracts['context'] = [' '.join(map(str, l)) for l in abstracts['context']]
abstracts.head(31)
```

```
[14]:                                              abstract  abstract_no  \
     0   inactivating mutations in the neurofibromatosi…         1406
     1   meningiomas constitute about 34% of primary in…         4003
     2   purpose: the purpose was to reevaluate in cell…          542
     3   neurofibromatosis type 2 ( nf2; mim # 101000) …         1549
     4   neurofibromatosis 2 (nf2) is a rare tumor supp…          355
     5   loss of the tumor suppressor merlin is a cause…          870
     6   loss of the tumor suppressor merlin is a cause…          870
     7   focal seizures are usually manifest with stere…         1970
     8   patients with neurofibromatosis type 1 (nf1) a…          595
     9   object. highgrade meningiomas in childhood are…          821
     10  objectives: spinal meningiomas mainly occur in…          903
     11  background: the pathogenesis of meningioma in …         1921
     12  introduction: minute pulmonary meningotheliall…         2267
     13  • aim: to investigate neurofibromatosis type 2…         2580
     14  opinion statement: neurofibromatosis type 1 (n…         4591
     15  neurofibromatosis type 2 (nf2) is an autosomal…          930
     16  meningiomas constitute about 34% of primary in…         4003
     17  purpose: the purpose was to reevaluate in cell…          542
     18  background. meningiomas are the most common pr…         2053
     19  patients with neurofibromatosis type 1 (nf1) a…          595
     20  purpose: to evaluate the mtorc1 (mammalian tar…            6
     21  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549
     22  purpose: to evaluate the mtorc1 (mammalian tar…            6
     23  loss of the tumor suppressor merlin causes dev…          683
     24  loss of the tumor suppressor merlin is a cause…          870
     25  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549
     26  purpose: the purpose was to reevaluate in cell…          542
     27  purpose: the purpose was to reevaluate in cell…          542
     28  methylation of the neurofibromatosis type 2 (n…         1499
     29  meningiomas are the most common primary intrac…         4490
     30  purpose: to evaluate the mtorc1 (mammalian tar…            6

                  drug   condition  \
     0          torin1  meningioma
     1            ar12  meningioma
     2       erlotinib  meningioma
     3       erlotinib  meningioma
     4     panobinostat  meningioma
     5       nilotinib  meningioma
     6     selumetinib  meningioma
     7    levetiracetam  meningioma
     8     doxorubicin  meningioma
     9     progesterone  meningioma
     10    progesterone  meningioma
     11    progesterone  meningioma
     12    progesterone  meningioma
```

```
13   progesterone  meningioma
14     lovastatin  meningioma
15           ar42  meningioma
16           ar42  meningioma
17      verapamil  meningioma
18      dasatinib  meningioma
19      etoposide  meningioma
20     everolimus  meningioma
21     everolimus  meningioma
22   temsirolimus  meningioma
23      sorafenib  meningioma
24      sorafenib  meningioma
25      sorafenib  meningioma
26    hydroxyurea  meningioma
27      tamoxifen  meningioma
28       cytidine  meningioma
29        azd2014  meningioma
30        uridine  meningioma

                                         abstract_norm  \
0   inactivating mutations in the neurofibromatosi…
1   meningiomas constitute about 34 of primary int…
2   purpose the purpose was to reevaluate in cell …
3   neurofibromatosis type 2  nf2 mim  101000 is a…
4   neurofibromatosis 2 nf2 is a rare tumor suppre…
5   loss of the tumor suppressor merlin is a becau…
6   loss of the tumor suppressor merlin is a becau…
7   focal seizures are usually manifest with stere…
8   patients with neurofibromatosis type 1 nf1 and…
9   object highgrade meningiomas in childhood are …
10  objectives spinal meningiomas mainly occur in …
11  background the pathogenesis of meningioma in f…
12  introduction minute pulmonary meningotheliali…
13   aim to investigate neurofibromatosis type 2 n…
14  opinion statement neurofibromatosis type 1 nf1…
15  neurofibromatosis type 2 nf2 is an autosomaldo…
16  meningiomas constitute about 34 of primary int…
17  purpose the purpose was to reevaluate in cell …
18  background meningiomas are the most common pri…
19  patients with neurofibromatosis type 1 nf1 and…
20  purpose to evaluate the mtorc1 mammalian targe…
21  neurofibromatosis type 2  nf2 mim  101000 is a…
22  purpose to evaluate the mtorc1 mammalian targe…
23  loss of the tumor suppressor merlin causes dev…
24  loss of the tumor suppressor merlin is a becau…
25  neurofibromatosis type 2  nf2 mim  101000 is a…
26  purpose the purpose was to reevaluate in cell …
```

```
27   purpose the purpose was to reevaluate in cell …
28   methylation of the neurofibromatosis type 2 nf…
29   meningiomas are the most common primary intrac…
30   purpose to evaluate the mtorc1 mammalian targe…

                                              context
0    profiles cells tumors finally examined rapamyc…
1    benmen1 cells addition decreased aurora b expr…
2    responses alkylating compound temozolomide var…
3    animal studies merlin pathway allowed biologic…
4    merlin deficient molecular phenotypes viabilit…
5    assays primary human vitro model tested pdgfrc…
6    concentrations lower steadystate trough plasma…
7    angiogram doppler carotid artery ultrasound sc…
8    p53 egf hdac well classical cytotoxic agents r…
9    extent surgery significantly related progressi…
10   li significantly higher values recurrent p 000…
11   females association exogenous remained unclear…
12   two mpmns revealed positive epithelial membran…
13   investigate type 2 gene mutation mrna levels s…
14   disorder may amenable treatment stimulant medi…
15   agent would inhibit vs simultaneously objectiv…
16   single nucleotide deletion exon 7 express prot…
17   alkylating compound temozolomide various drugs…
18   eph rtks ckit src family kinase sfk members bi…
19   p53 egf hdac well classical cytotoxic agents r…
20   mtorc1 pathway expressed activated independent…
21   animal studies merlin pathway allowed biologic…
22   assess sensitivity toward mtorc1 inhibitors me…
23   overexpressionactivation plateletderived growt…
24   kinase erk12 akt increased growth successfully…
25   merlin pathway allowed biologically targeted t…
26   specifically separate death pure inhibition pr…
27   responses alkylating compound temozolomide var…
28   dnmt1 cells dnmt13b leptomeningeal cells upreg…
29   sgk1 rescues mtorc1 activation sgk1 activation…
30   merlinpositive negative cells used assess sens…
```

4.4 Tokenize

[15]:
```
abstracts['tokenized'] = abstracts['context'].apply(lambda x : nltk.
 ↪word_tokenize(x))
abstracts.head(3)
```

[15]:
```
                                            abstract  abstract_no      drug  \
0  inactivating mutations in the neurofibromatosi…         1406    torin1
1  meningiomas constitute about 34% of primary in…         4003      ar12
```

```
2  purpose: the purpose was to reevaluate in cell…         542  erlotinib

    condition                                      abstract_norm  \
0  meningioma  inactivating mutations in the neurofibromatosi…
1  meningioma  meningiomas constitute about 34 of primary int…
2  meningioma  purpose the purpose was to reevaluate in cell …

                                             context  \
0  profiles cells tumors finally examined rapamyc…
1  benmen1 cells addition decreased aurora b expr…
2  responses alkylating compound temozolomide var…

                                           tokenized
0  [profiles, cells, tumors, finally, examined, r…
1  [benmen1, cells, addition, decreased, aurora, …
2  [responses, alkylating, compound, temozolomide…
```

4.5 Lemmatize

[16]:

```
#step 1
abstracts['pos_tags'] = abstracts['tokenized'].apply(nltk.tag.pos_tag)

#step 2
def get_wordnet_pos(tag):
    if tag.startswith('J'):
        return wordnet.ADJ
    elif tag.startswith('V'):
        return wordnet.VERB
    elif tag.startswith('N'):
        return wordnet.NOUN
    elif tag.startswith('R'):
        return wordnet.ADV
    else:
        return wordnet.NOUN

#step 3
abstracts['wordnet_pos'] = abstracts['pos_tags'].apply(lambda x: [(word,␣
 ↪get_wordnet_pos(pos_tag)) for (word, pos_tag) in x])

#step 4
wnl = WordNetLemmatizer()
abstracts['lemmatized'] = abstracts['wordnet_pos'].apply(lambda x: [wnl.
 ↪lemmatize(word, tag) for word, tag in x])
```

[17]:

```
# 'lemmatized' needs to be a string
abstracts['lemmatized_str'] = [' '.join(map(str, l)) for l in␣
 ↪abstracts['lemmatized']]
```

```
abstracts.head(3)
```

```
[17]:
                                          abstract  abstract_no       drug  \
0  inactivating mutations in the neurofibromatosi…         1406     torin1
1  meningiomas constitute about 34% of primary in…         4003       ar12
2  purpose: the purpose was to reevaluate in cell…          542  erlotinib

    condition                                    abstract_norm  \
0  meningioma  inactivating mutations in the neurofibromatosi…
1  meningioma  meningiomas constitute about 34 of primary int…
2  meningioma  purpose the purpose was to reevaluate in cell …

                                           context  \
0  profiles cells tumors finally examined rapamyc…
1  benmen1 cells addition decreased aurora b expr…
2  responses alkylating compound temozolomide var…

                                         tokenized  \
0  [profiles, cells, tumors, finally, examined, r…
1  [benmen1, cells, addition, decreased, aurora, …
2  [responses, alkylating, compound, temozolomide…

                                          pos_tags  \
0  [(profiles, NNS), (cells, NNS), (tumors, NNS),…
1  [(benmen1, NN), (cells, NNS), (addition, NN), …
2  [(responses, NNS), (alkylating, VBG), (compoun…

                                       wordnet_pos  \
0  [(profiles, n), (cells, n), (tumors, n), (fina…
1  [(benmen1, n), (cells, n), (addition, n), (dec…
2  [(responses, n), (alkylating, v), (compound, n…

                                        lemmatized  \
0  [profile, cell, tumor, finally, examine, rapam…
1  [benmen1, cell, addition, decrease, aurora, b,…
2  [response, alkylating, compound, temozolomide,…

                                    lemmatized_str
0  profile cell tumor finally examine rapamycin w…
1  benmen1 cell addition decrease aurora b expres…
2  response alkylating compound temozolomide vari…
```

4.6 Combine with disease summary and abstract dataframes

4.6.1 Add pair column to merge on

```
[18]: abstracts['pair'] = list(zip(abstracts.drug, abstracts.condition))
      disease_summary['pair'] = list(zip(disease_summary.drug, disease_summary.
       ↪condition))
```

4.6.2 Create df that combines abstracts of all drug-condition pairs

```
[19]: #How many unique drug-condition pairs do we have?
      df = pd.DataFrame(abstracts.groupby(['drug', 'condition']).size().
       ↪reset_index(name='Freq'))
      df['pair'] = list(zip(df.drug, df.condition))
      df.head()
```

```
[19]:       drug   condition  Freq                   pair
      0     ar12  meningioma     1     (ar12, meningioma)
      1     ar42  meningioma     2     (ar42, meningioma)
      2     ar42  schwannoma     2     (ar42, schwannoma)
      3  aspirin  schwannoma     2  (aspirin, schwannoma)
      4  azd2014  meningioma     1  (azd2014, meningioma)
```

```
[20]: no_abs = []
      len_no_abs = []
      counts_context = []

      for a in range(len(df.pair)):
          temp = pd.DataFrame(abstracts[df.pair[a] == abstracts.pair])

          ## add abstract numbers
          abs_no = temp.abstract_no.tolist()
          no_abs.append(abs_no)

          ## add total number of abstracts
          abs_len = len(abs_no)
          len_no_abs.append(abs_len)

          ##retain counts and do not remove duplicates
          counts = temp.lemmatized_str.tolist()
          counts = ' '.join(counts)
          counts = counts.split()
          counts = ' '.join(counts)
          counts_context.append(counts)
```

```
[21]: df["abs_no"] = no_abs
      df["abs_len"] = len_no_abs
```

```
df["words"] = counts_context

df.head()
```

```
[21]:      drug   condition  Freq                  pair        abs_no  abs_len  \
      0     ar12  meningioma     1     (ar12, meningioma)        [4003]        1
      1     ar42  meningioma     2     (ar42, meningioma)   [930, 4003]        2
      2     ar42  schwannoma     2     (ar42, schwannoma)   [930, 2867]        2
      3  aspirin  schwannoma     2  (aspirin, schwannoma)  [3567, 3792]        2
      4  azd2014  meningioma     1  (azd2014, meningioma)        [4490]        1

                                                   words
      0  benmen1 cell addition decrease aurora b expres…
      1  agent would inhibit vs simultaneously objectiv…
      2  agent would inhibit vs simultaneously objectiv…
      3  major abnormality strikingly treatment tumorde…
      4  sgk1 rescue mtorc1 activation sgk1 activation …
```

4.6.3 Merge dataframes

```
[22]: ## avoid duplicated drug and condition columns
      columns=['drug', 'condition']

      ## merge data frames
      merged_data = df.merge(disease_summary.drop(columns,1), how = 'inner', on =␣
       ↪['pair'])

      ## what are we working with
      merged_data.head(3)
```

```
[22]:   drug   condition  Freq                pair       abs_no  abs_len  \
      0  ar12  meningioma     1  (ar12, meningioma)       [4003]        1
      1  ar42  meningioma     2  (ar42, meningioma)  [930, 4003]        2
      2  ar42  schwannoma     2  (ar42, schwannoma)  [930, 2867]        2

                                                   words    median      mean  \
      0  benmen1 cell addition decrease aurora b expres…  1.148433  1.103720
      1  agent would inhibit vs simultaneously objectiv…  0.843940  0.613611
      2  agent would inhibit vs simultaneously objectiv…  0.191010  0.374396

              min       max disease_name
      0  0.822028  1.273501          NF2
      1  0.000323  1.157063          NF2
      2  0.001217  1.175912          NF2
```

```
[23]: merged_data.loc[merged_data['drug'] == "mycophenolate mofetil"]
```

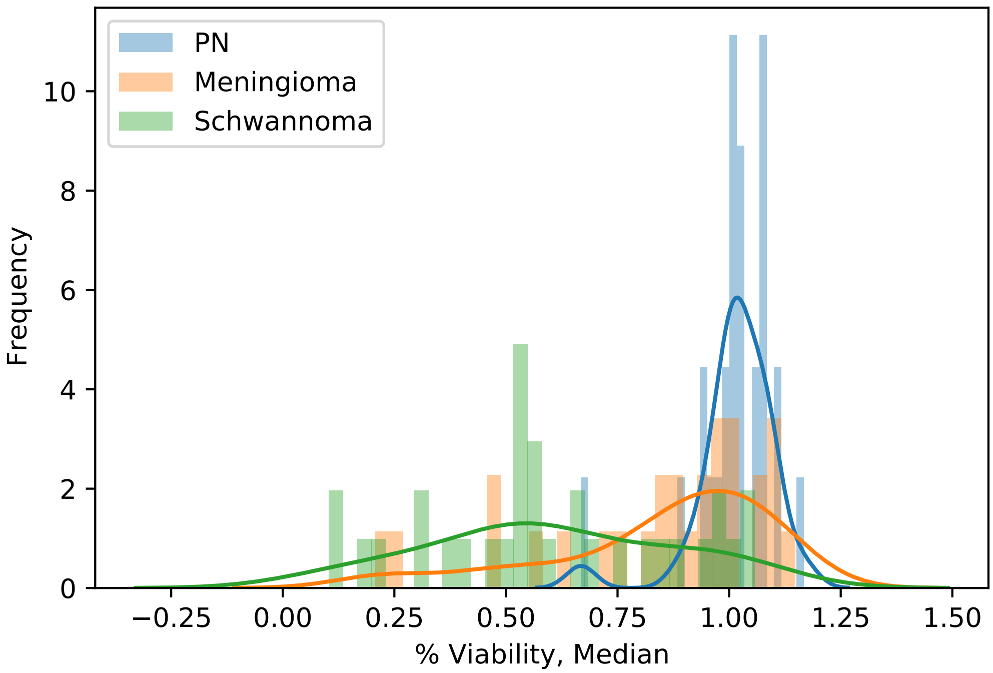
```
[23]:                       drug condition  Freq                            pair  \
      45  mycophenolate mofetil       pNF     1  (mycophenolate mofetil, pNF)

          abs_no  abs_len                                             words  \
      45  [4714]        1  extensive hematoma right side cta maintenance …

            median     mean       min       max disease_name
      45  1.056076  0.99374  0.291549  1.303233          NF1
```

```
[24]: print(merged_data.shape)
      print(merged_data.Freq.sum())
```

```
(87, 12)
144
```

4.6.4 Histograms by condition

```
[25]: sns.distplot(merged_data[(merged_data.condition == 'pNF')].loc[:, 'median'],␣
       ↪bins = 30);
      sns.distplot(merged_data[(merged_data.condition == 'meningioma')].loc[:,␣
       ↪'median'], bins = 30);
      sns.distplot(merged_data[(merged_data.condition == 'schwannoma')].loc[:,␣
       ↪'median'], bins = 30);
      plt.legend(['PN', 'Meningioma', 'Schwannoma']);
      plt.xlabel('% Viability, Median');
      plt.ylabel('Frequency');

      plt.savefig("../images/Fig4.png", dpi=410);
```

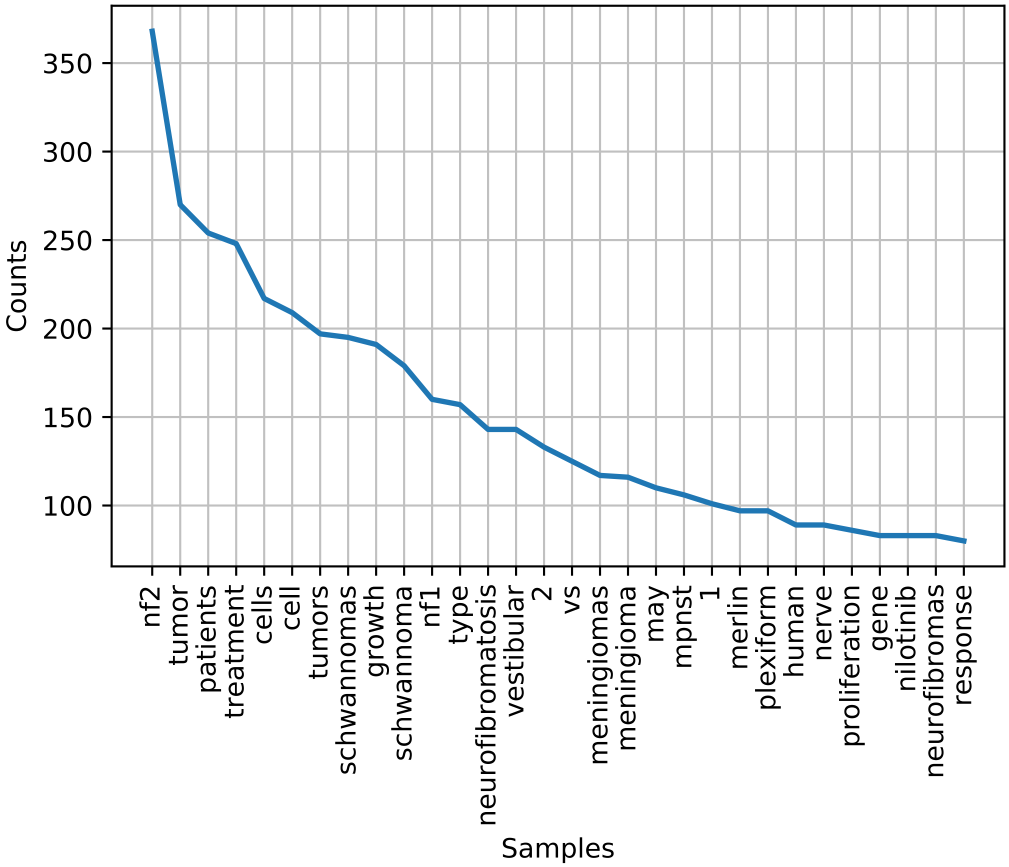


4.6.5 Compare stopwords using wordcloud

Original stopword dictionary plus no +/- 10 words

[26]:
```
stop_words = set(stopwords.words('english'))

temp = abstracts['abstract_norm'].apply(lambda x : nltk.word_tokenize(x))
stopword_test = temp.apply(lambda x: [word for word in x if word not in␣
 ↪stop_words])

stopword_test = stopword_test.apply(lambda x: ' '.join(x))
```

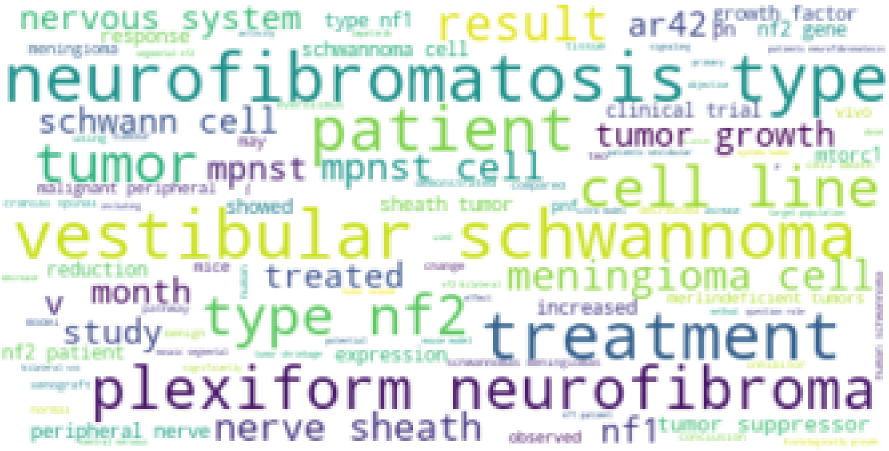
[27]:
```
txt = stopword_test.str.replace(r'\|', ' ').str.cat(sep=' ')
words = nltk.tokenize.word_tokenize(txt)
word_dist = nltk.FreqDist(words)

fig = plt.figure(figsize = (6,4))
plt.gcf().subplots_adjust(bottom=0.15) # to avoid x-ticks cut-off

## show 30 most frequent words
word_dist.plot(30,cumulative=False);

plt.show();
fig.savefig("../images/Fig5a1.png", bbox_inches = "tight")
```



```
[28]: #The top 100 words
      rslt = pd.DataFrame(word_dist.most_common(100), columns=['Word', 'Frequency'])
      display(rslt)
```

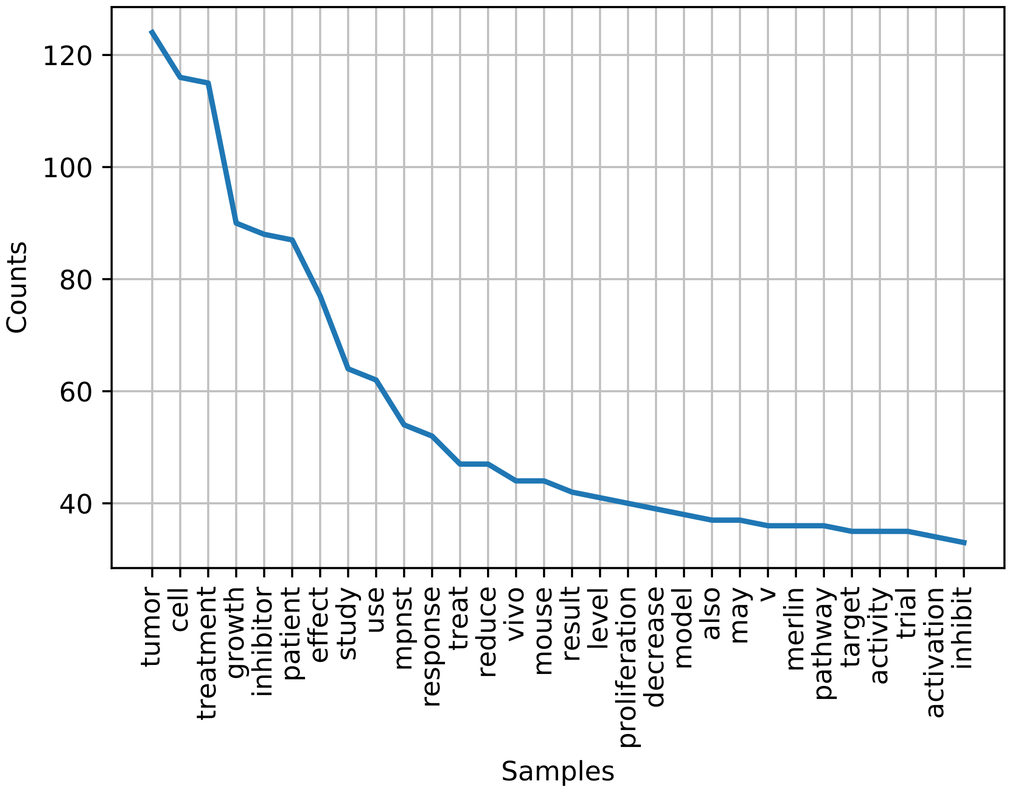
```
            Word  Frequency
0            nf2        368
1          tumor        270
2       patients        254
3      treatment        248
4          cells        217
..           ...        ...
95           one         44
96          data         43
97    inhibition         42
98       surgery         42
99           akt         41

[100 rows x 2 columns]
```

[29]:
```
wordcloud = WordCloud(max_font_size=50, max_words=100,␣
 ↪background_color="white").generate(txt)
plt.figure();
plt.imshow(wordcloud, interpolation="bilinear");
plt.axis("off");

plt.savefig("../images/Fig5a2.png", dpi=410);
plt.show();
```



Augmented stopword dictionary

[30]:
```
txt = merged_data.words.str.replace(r'\|', ' ').str.cat(sep=' ')
words = nltk.tokenize.word_tokenize(txt)
word_dist = nltk.FreqDist(words)

fig = plt.figure(figsize = (6,4))
plt.gcf().subplots_adjust(bottom=0.15) # to avoid x-ticks cut-off

## show 30 most frequent words
word_dist.plot(30,cumulative=False);

plt.show();
fig.savefig("../images/Fig5b1.png", bbox_inches = "tight")
```

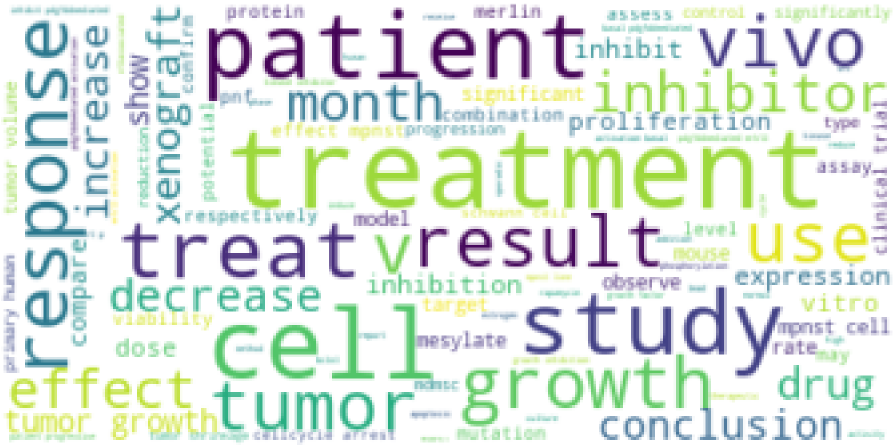


```
[31]: #The top 100 words
      rslt = pd.DataFrame(word_dist.most_common(100), columns=['Word', 'Frequency'])
      display(rslt)
```

```
                  Word  Frequency
0                tumor        124
1                 cell        116
2            treatment        115
3               growth         90
4            inhibitor         88
..                 ...        ...
95             schwann         15
96              assess         15
97   4hydroxytamoxifen         15
98               basal         15
99               cycle         14

[100 rows x 2 columns]
```

```
[32]: wordcloud = WordCloud(max_font_size=50, max_words=100,␣
       ↪background_color="white").generate(txt)
```

```
plt.figure();
plt.imshow(wordcloud, interpolation="bilinear");
plt.axis("off");

plt.savefig("../images/Fig5b2.png", dpi=410);
plt.show();
```



5 Split into "training" and "testing" data

[33]:
```
train_data = merged_data[merged_data['condition'] != 'pNF']
test_data = merged_data[merged_data['condition'] == 'pNF']
```

[34]:
```
print(train_data.shape)
print(test_data.shape)
```

```
(60, 12)
(27, 12)
```

6 Create text representation

[35]:
```
def make_bow(train, test, M_set=0.1, bin_set=True):
    #vocab = None

    tf_vectorizer_bin = CountVectorizer(binary=bin_set, min_df=M_set)

    tf_train = tf_vectorizer_bin.fit_transform(train)
    tf_feature_names = tf_vectorizer_bin.get_feature_names() #bag of vocabulary
    Train_BoW = tf_train.toarray()
    matrix_train = pd.DataFrame(Train_BoW, columns=list(tf_feature_names))
    tf_test = tf_vectorizer_bin.transform(test)
    Test_BoW = tf_test.toarray()
    matrix_test = pd.DataFrame(Test_BoW, columns=list(tf_feature_names))

    return matrix_train, matrix_test, tf_feature_names
```

Adapted from here

[36]:

```
def run_pca(input_mx, target_vx, pc=2):

    pca = PCA(n_components=pc)

    principalComponents = pca.fit_transform(input_mx)

    pc_labels = ['PC'+str(i) for i in range(1, pc+1)]
    df_pca = pd.DataFrame(data = principalComponents,
                          columns = pc_labels)
    df_pca.reset_index(drop=True, inplace=True)

    target = target_vx
    target.reset_index(drop=True, inplace=True)

    df_pca = pd.concat([df_pca, target], axis = 1)

    return df_pca
```

6.1 Bag-of-words: binary matrix

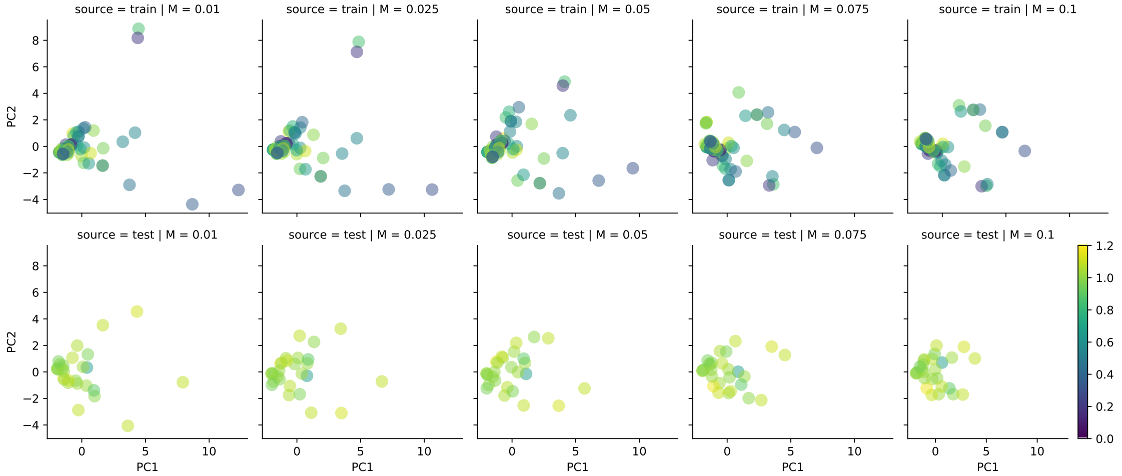
[37]:

```
m_list = [0.01, 0.025, 0.05, 0.075, 0.1]

PC1_train_list = []
PC2_train_list = []
PC3_train_list = []
train_med_list = []

PC1_test_list = []
PC2_test_list = []
PC3_test_list = []
test_med_list = []

## create lists of PCs given different M values
for m in m_list:

    ## features not in use here
    matrix_train_count, matrix_test_count, features =␣
 ↪make_bow(train_data['words'], test_data['words'],
                                                              M_set = m,␣
 ↪bin_set = True)

    df_pca_train = run_pca(matrix_train_count, train_data[['median']], pc=3)
    df_pca_test = run_pca(matrix_test_count, test_data[['median']], pc=3)

    PC1_train_list.extend(df_pca_train.PC1)
    PC2_train_list.extend(df_pca_train.PC2)
    PC3_train_list.extend(df_pca_train.PC3)
    train_med_list.extend(df_pca_train['median'])

    PC1_test_list.extend(df_pca_test.PC1)
    PC2_test_list.extend(df_pca_test.PC2)
    PC3_test_list.extend(df_pca_test.PC3)
    test_med_list.extend(df_pca_test['median'])

## create dataframes for training data
m_labs_train = [[i]*len(train_data[['median']]) for i in m_list]
m_labs_train = [item for sublist in m_labs_train for item in sublist]

df_pca_train = pd.DataFrame(data = {'PC1': PC1_train_list,
                                    'PC2': PC2_train_list,
                                    'PC3': PC3_train_list,
                                    'median': train_med_list,
                                    'M': m_labs_train})
df_pca_train.reset_index(drop=True, inplace=True)

## create dataframes for testing data
m_labs_test = [[i]*len(test_data[['median']]) for i in m_list]
m_labs_test = [item for sublist in m_labs_test for item in sublist]

df_pca_test = pd.DataFrame(data = {'PC1': PC1_test_list,
                                   'PC2': PC2_test_list,
                                   'PC3': PC3_test_list,
                                   'median': test_med_list,
                                   'M': m_labs_test})
df_pca_test.reset_index(drop=True, inplace=True)

df_pca = pd.concat([df_pca_train, df_pca_test], axis = 0)

df_pca['source'] = ['train']*df_pca_train.shape[0] + ['test']*df_pca_test.
 ↪shape[0]
```

Adapted from here

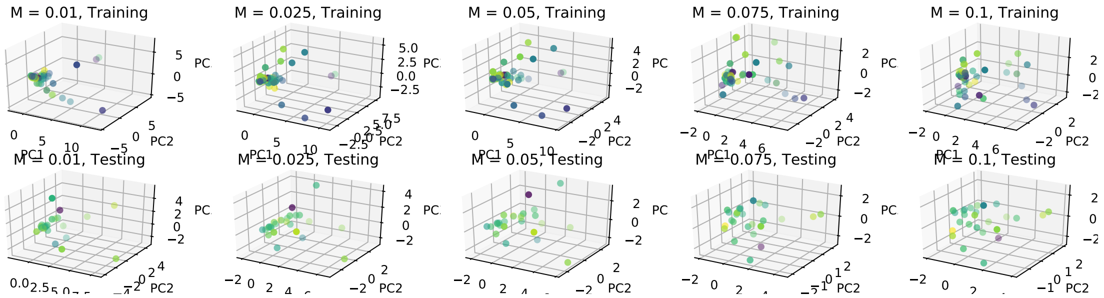
```
[38]: g = sns.FacetGrid(df_pca, row = 'source', col = 'M', palette = 'seismic');
```

```python
def facet_scatter(x, y, c, **kwargs):
    kwargs.pop("color")
    plt.scatter(x, y, c=c, **kwargs)

vmin, vmax = 0, 1.2
cmap = plt.cm.viridis

norm=plt.Normalize(vmin=vmin, vmax=vmax)

g = g.map(facet_scatter, 'PC1', 'PC2', 'median',
          s=100, alpha=0.5, norm=norm, cmap=cmap)

# Make space for the colorbar
g.fig.subplots_adjust(right=.9)

points = plt.scatter([], [], c=[], vmin=vmin, vmax=vmax, cmap=cmap)
g.fig.colorbar(points)

plt.savefig("../images/Fig6a1.png", dpi=410);
plt.show();
```



[39]:

```python
fig = plt.figure(figsize=plt.figaspect(0.25))

for i, j in enumerate(m_list):
    ax = fig.add_subplot(2, len(m_list), i+1, projection='3d')

    ax.set_xlabel('PC1')
    ax.set_ylabel('PC2')
    ax.set_zlabel('PC3')
    ax.set_title('M = ' + str(j) + ', Training')
    ax.scatter(df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'PC1'],
               df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'PC2'],
               df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'PC3'],
               c=df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'median'],
               marker='o',
               cmap=plt.cm.viridis);

for i, j in enumerate(m_list):
    ax = fig.add_subplot(2, len(m_list), i+6, projection='3d')

    ax.set_xlabel('PC1')
    ax.set_ylabel('PC2')
    ax.set_zlabel('PC3')
    ax.set_title('M = ' + str(j) + ', Testing')

    ax.scatter(df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)), 'PC1'],
               df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)), 'PC2'],
               df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)), 'PC3'],
               c=df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)),␣
 ↪'median'],
               marker='o',
               cmap=plt.cm.viridis);

plt.savefig("../images/Fig6a2.png", dpi=410);
plt.show();
```



[40]:
```
dist = DistanceMetric.get_metric('euclidean')

for m in m_list:
    df_m = df_pca.loc[((df_pca.M == m) & (df_pca.source == 'train')), ['PC1',␣
↪'PC2', 'PC3']]
    df_m = np.array(df_m)
    mx_dist_bin = dist.pairwise(df_m)
    avg = np.mean(np.triu(mx_dist_bin, k = 1))
    sd = np.std(np.triu(mx_dist_bin, k = 1))

    print('The average distance for M = ' + str(m) + ' is ' + str(avg))
    print('The standard deviation distance for M = ' + str(m) + ' is ' +␣
↪str(sd))
    print()
```

```
The average distance for M = 0.01 is 1.6649892942451614
The standard deviation distance for M = 0.01 is 3.1091165819127995

The average distance for M = 0.025 is 1.6762834910236106
The standard deviation distance for M = 0.025 is 2.8535287775203653

The average distance for M = 0.05 is 1.6907233930289631
The standard deviation distance for M = 0.05 is 2.5882833615514

The average distance for M = 0.075 is 1.5455754785828282
The standard deviation distance for M = 0.075 is 2.1807137506101144

The average distance for M = 0.1 is 1.4476892032247095
The standard deviation distance for M = 0.1 is 2.088306699672119
```

[41]:
```
matrix_train_bin, matrix_test_bin, features_bin = make_bow(train_data['words'],␣
↪test_data['words'],
                                                           M_set = 0.05,␣
↪bin_set = True)
matrix_train_bin.head(5)
```

[41]:
```
   00001  10  14  20  2011  40  908  achievable  across  activation  …  \
0      0   0   0   0     0   0    0           0       0           0  …
1      0   1   0   0     1   0    0           0       0           1  …
2      0   1   0   0     1   0    0           0       0           1  …
3      0   0   0   0     0   0    0           0       0           0  …
4      0   0   0   0     0   0    0           0       0           1  …

   volumetric  vs  way  weight  well  western  whereas  whether  without  \
0           0   0    0       0     0        0        0        0        0
1           1   1    0       0     0        1        1        0        0
2           1   1    0       1     0        1        0        1        0
3           0   0    0       0     0        0        0        0        0
4           0   0    0       0     0        0        0        0        0
```

```
   xenograft
0          1
1          1
2          1
3          0
4          0

[5 rows x 322 columns]
```

[42]:

```
X_train_bin = matrix_train_bin
X_train_bin['freq'] = list(train_data['Freq'])

X_test_bin = matrix_test_bin
X_test_bin['freq'] = list(test_data['Freq'])
```

6.2 Bag-of-words: count matrix

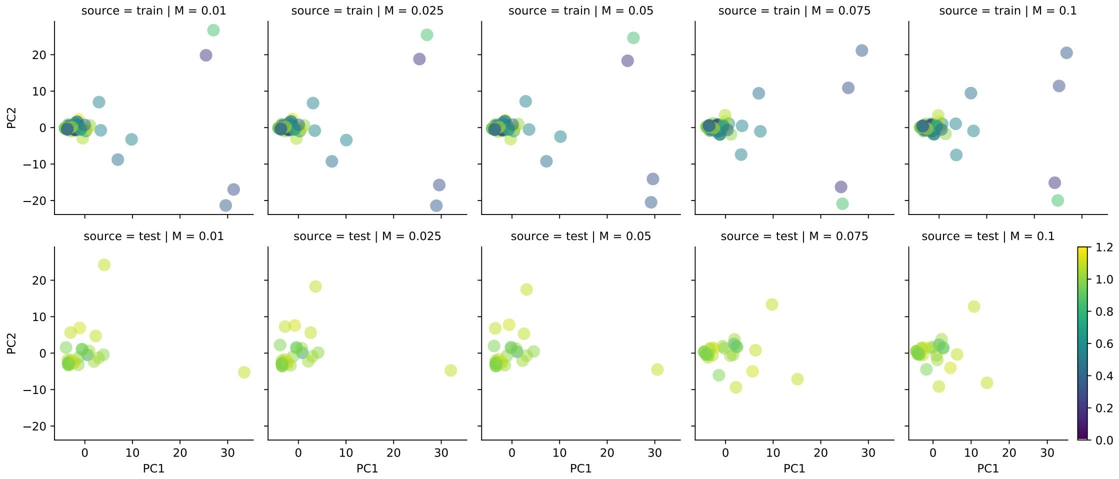
[43]:

```
m_list = [0.01, 0.025, 0.05, 0.075, 0.1]

PC1_train_list = []
PC2_train_list = []
PC3_train_list = []
train_med_list = []

PC1_test_list = []
PC2_test_list = []
PC3_test_list = []
test_med_list = []

## create lists of PCs given different M values
for m in m_list:

    ## features not in use here
    matrix_train_count, matrix_test_count, features =␣
 ↪make_bow(train_data['words'], test_data['words'],
                                                            M_set = m,␣
 ↪bin_set = False)

    df_pca_train = run_pca(matrix_train_count, train_data[['median']], pc=3)
    df_pca_test = run_pca(matrix_test_count, test_data[['median']], pc=3)

    PC1_train_list.extend(df_pca_train.PC1)
    PC2_train_list.extend(df_pca_train.PC2)
    PC3_train_list.extend(df_pca_train.PC3)
    train_med_list.extend(df_pca_train['median'])
    PC1_test_list.extend(df_pca_test.PC1)
    PC2_test_list.extend(df_pca_test.PC2)
    PC3_test_list.extend(df_pca_test.PC3)
    test_med_list.extend(df_pca_test['median'])

## create dataframes for training data
m_labs_train = [[i]*len(train_data[['median']]) for i in m_list]
m_labs_train = [item for sublist in m_labs_train for item in sublist]

df_pca_train = pd.DataFrame(data = {'PC1': PC1_train_list,
                                    'PC2': PC2_train_list,
                                    'PC3': PC3_train_list,
                                    'median': train_med_list,
                                    'M': m_labs_train})
df_pca_train.reset_index(drop=True, inplace=True)

## create dataframes for testing data
m_labs_test = [[i]*len(test_data[['median']]) for i in m_list]
m_labs_test = [item for sublist in m_labs_test for item in sublist]

df_pca_test = pd.DataFrame(data = {'PC1': PC1_test_list,
                                   'PC2': PC2_test_list,
                                   'PC3': PC3_test_list,
                                   'median': test_med_list,
                                   'M': m_labs_test})
df_pca_test.reset_index(drop=True, inplace=True)

df_pca = pd.concat([df_pca_train, df_pca_test], axis = 0)

df_pca['source'] = ['train']*df_pca_train.shape[0] + ['test']*df_pca_test.
 ↪shape[0]
```

[44]:

```
g = sns.FacetGrid(df_pca, row = 'source', col = 'M', palette = 'seismic');

def facet_scatter(x, y, c, **kwargs):
    kwargs.pop("color")
    plt.scatter(x, y, c=c, **kwargs)

vmin, vmax = 0, 1.2
cmap = plt.cm.viridis

norm=plt.Normalize(vmin=vmin, vmax=vmax)

g = g.map(facet_scatter, 'PC1', 'PC2', 'median',
          s=100, alpha=0.5, norm=norm, cmap=cmap)
```

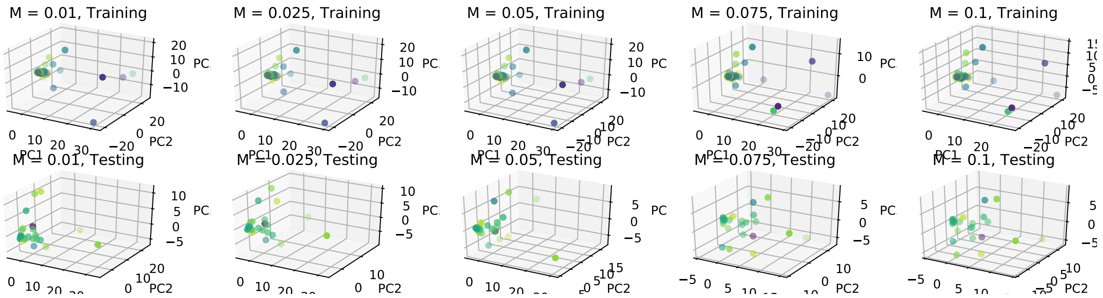
```
# Make space for the colorbar
g.fig.subplots_adjust(right=.9)

points = plt.scatter([], [], c=[], vmin=vmin, vmax=vmax, cmap=cmap)
g.fig.colorbar(points)

plt.savefig("../images/Fig6b1.png", dpi=410);
plt.show();
```



[45]:

```
fig = plt.figure(figsize=plt.figaspect(0.25))

for i, j in enumerate(m_list):
    ax = fig.add_subplot(2, len(m_list), i+1, projection='3d')

    ax.set_xlabel('PC1')
    ax.set_ylabel('PC2')
    ax.set_zlabel('PC3')
    ax.set_title('M = ' + str(j) + ', Training')

    ax.scatter(df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'PC1'],
               df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'PC2'],
               df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'PC3'],
               c=df_pca.loc[((df_pca.source == 'train') & (df_pca.M == j)),␣
 ↪'median'],
               marker='o',
               cmap=plt.cm.viridis);
```

```
for i, j in enumerate(m_list):
    ax = fig.add_subplot(2, len(m_list), i+6, projection='3d')

    ax.set_xlabel('PC1')
    ax.set_ylabel('PC2')
    ax.set_zlabel('PC3')
    ax.set_title('M = ' + str(j) + ', Testing')

    ax.scatter(df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)), 'PC1'],
               df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)), 'PC2'],
               df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)), 'PC3'],
               c=df_pca.loc[((df_pca.source == 'test') & (df_pca.M == j)),␣
 ↪'median'],
               marker='o',
               cmap=plt.cm.viridis);

plt.savefig("../images/Fig6b2.png", dpi=410);
plt.show();
```



[46]:
```
dist = DistanceMetric.get_metric('euclidean')

for m in m_list:
    df_m = df_pca.loc[((df_pca.M == m) & (df_pca.source == 'train')), ['PC1',␣
 ↪'PC2', 'PC3']]
    df_m = np.array(df_m)
    mx_dist_bin = dist.pairwise(df_m)
    avg = np.mean(np.triu(mx_dist_bin, k = 1))
    sd = np.std(np.triu(mx_dist_bin, k = 1))

    print('The average distance for M = ' + str(m) + ' is ' + str(avg))
    print('The standard deviation distance for M = ' + str(m) + ' is ' +␣
 ↪str(sd))
    print()
```

```
The average distance for M = 0.01 is 4.267897959281668
The standard deviation distance for M = 0.01 is 9.941865383562257
The average distance for M = 0.025 is 4.238358097718487
The standard deviation distance for M = 0.025 is 9.666328010577873

The average distance for M = 0.05 is 4.184160447162683
The standard deviation distance for M = 0.05 is 9.419381224258139

The average distance for M = 0.075 is 3.8730059013992
The standard deviation distance for M = 0.075 is 8.570780844195514

The average distance for M = 0.1 is 3.809321532603673
The standard deviation distance for M = 0.1 is 8.352448082464626
```

[47]:

```
matrix_train_count, matrix_test_count, features_count =␣
 ↪make_bow(train_data['words'], test_data['words'],
                                                  M_set = 0.01,␣
 ↪bin_set = False)
matrix_train_count.shape
matrix_train_count.head(5)
```

[47]:

```
   00001  00025  00062  0009  001  0038  005  05  0969  09748  …  whether  \
0      0      0      0     0    0     0    0   0     0      0  …        0
1      0      0      0     0    0     0    0   0     0      0  …        0
2      0      0      0     0    0     0    0   0     0      0  …        2
3      0      0      0     0    0     0    0   0     0      0  …        0
4      0      0      0     0    0     0    0   0     0      0  …        0

   wildtype  within  without  would  xenograft  xenograftbearing  xenografts  \
0         0       0        0      0          2                 0           0
1         0       0        0      1          4                 2           2
2         2       0        0      1          3                 0           2
3         0       0        0      0          0                 0           0
4         0       0        0      0          0                 0           0

   year  young
0     0      0
1     0      0
2     0      0
3     0      0
4     0      0

[5 rows x 1024 columns]
```

[48]:

```
X_train_count = matrix_train_count
X_train_count['freq'] = list(train_data['Freq'])
```

```
X_test_count = matrix_test_count
X_test_count['freq'] = list(test_data['Freq'])
```

6.3 TF-IDF

[49]:

```
#same vocabulary
vocabulary = features_bin
abstracts_train = train_data.words.tolist()
abstracts_test = test_data.words.tolist()
```

[50]:

```
#Calculate TF-IDF
def calc_TF(vocab, docs):
    tfDict = {}
    for word in vocab:
        tf_per_word = []
        for doc in docs:
            length = len(doc.split())
            count = doc.split().count(word)
            freq = (count/length)
            tf_per_word.append(freq)
        tfDict[word] = tf_per_word
    return tfDict

def calc_IDF(vocab, docs):
    N = len(docs)
    idfDict = {}
    for word in vocab:
        counts = 0
        for doc in docs:
            if word in (doc.split()):
                counts += 1
        idfDict[word] = np.log(N/(counts+1)) #shouldnt be +1, but a solution␣
 ↪online to how testing data might not have that word
    return idfDict

def calc_TF_IDF(vocab, docs):
    tfDict = calc_TF(vocab, docs)
    idfDict = calc_IDF(vocab, docs)
    tfidf_values = []
    for word in tfDict.keys():
        tfidf_abstracts = []
        for abst in tfDict[word]:
            tf_idf_score = abst * idfDict[word]
            tfidf_abstracts.append(tf_idf_score)
        tfidf_values.append(tfidf_abstracts)
    return tfidf_values
```

```
[51]: tfidf_train = calc_TF_IDF(vocabulary, abstracts_train)
      tfidf_train_model = np.asarray(tfidf_train)
      tfidf_train_model = tfidf_train_model.T
      tfidf_train_model.shape
```

```
[51]: (60, 322)
```

```
[52]: matrix_train_tfidf = pd.DataFrame(tfidf_train_model)
      matrix_train_tfidf.columns = matrix_train_bin.drop(columns='freq').columns
      matrix_train_tfidf.head()
```

```
[52]:    00001        10   14   20      2011   40  908  achievable  across  \
      0    0.0  0.000000  0.0  0.0  0.000000  0.0  0.0         0.0     0.0
      1    0.0  0.005916  0.0  0.0  0.012895  0.0  0.0         0.0     0.0
      2    0.0  0.006212  0.0  0.0  0.013540  0.0  0.0         0.0     0.0
      3    0.0  0.000000  0.0  0.0  0.000000  0.0  0.0         0.0     0.0
      4    0.0  0.000000  0.0  0.0  0.000000  0.0  0.0         0.0     0.0

         activation  …  volumetric        vs  way   weight  well   western  \
      0    0.000000  …    0.000000  0.000000  0.0  0.00000   0.0  0.000000
      1    0.012798  …    0.011833  0.009595  0.0  0.00000   0.0  0.011833
      2    0.013438  …    0.012425  0.020149  0.0  0.01354   0.0  0.012425
      3    0.000000  …    0.000000  0.000000  0.0  0.00000   0.0  0.000000
      4    0.049089  …    0.000000  0.000000  0.0  0.00000   0.0  0.000000

          whereas  whether  without  xenograft
      0  0.000000  0.00000      0.0   0.115129
      1  0.012895  0.00000      0.0   0.021929
      2  0.000000  0.01354      0.0   0.017269
      3  0.000000  0.00000      0.0   0.000000
      4  0.000000  0.00000      0.0   0.000000

      [5 rows x 322 columns]
```

```
[53]: tfidf_test = calc_TF_IDF(vocabulary, abstracts_test)
      tfidf_test_model = np.asarray(tfidf_test)
      tfidf_test_model = tfidf_test_model.T
      tfidf_test_model.shape
```

```
[53]: (27, 322)
```

```
[54]: matrix_test_tfidf = pd.DataFrame(tfidf_test_model)
      matrix_test_tfidf.columns = matrix_test_bin.drop(columns='freq').columns
      matrix_test_tfidf.head()
```

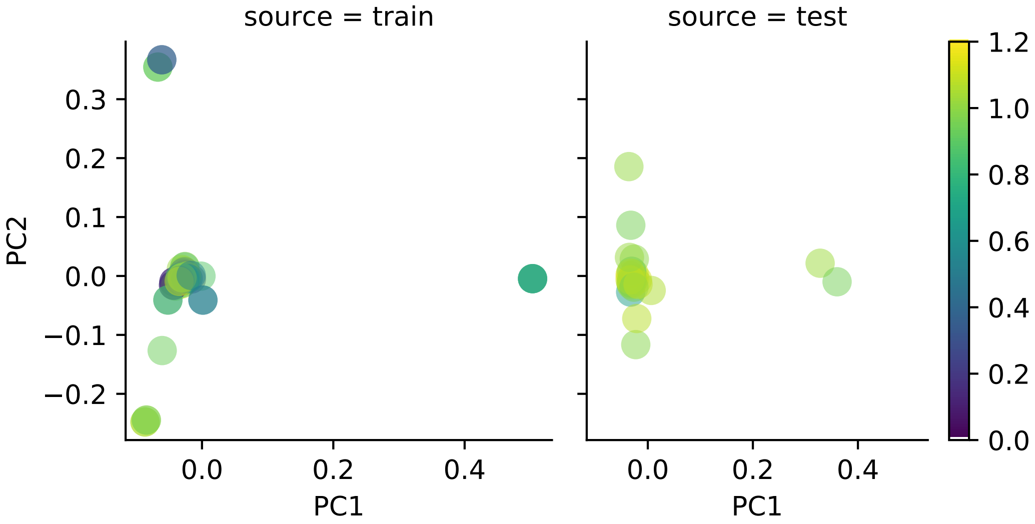
```
[54]:    00001   10   14   20  2011   40  908  achievable  across  activation  …  \
      0    0.0  0.0  0.0  0.0   0.0  0.0  0.0         0.0     0.0         0.0  …
```

```
1    0.0  0.0  0.0  0.0   0.0  0.0  0.0         0.0     0.0         0.0  …
2    0.0  0.0  0.0  0.0   0.0  0.0  0.0         0.0     0.0         0.0  …
3    0.0  0.0  0.0  0.0   0.0  0.0  0.0         0.0     0.0         0.0  …
4    0.0  0.0  0.0  0.0   0.0  0.0  0.0         0.0     0.0         0.0  …

   volumetric   vs  way  weight      well  western  whereas   whether  \
0         0.0  0.0  0.0     0.0  0.010227  0.000000      0.0  0.000000
1         0.0  0.0  0.0     0.0  0.000000  0.016684      0.0  0.012241
2         0.0  0.0  0.0     0.0  0.000000  0.000000      0.0  0.000000
3         0.0  0.0  0.0     0.0  0.000000  0.000000      0.0  0.000000
4         0.0  0.0  0.0     0.0  0.000000  0.000000      0.0  0.000000

    without  xenograft
0  0.000000        0.0
1  0.014085        0.0
2  0.000000        0.0
3  0.000000        0.0
4  0.000000        0.0

[5 rows x 322 columns]
```

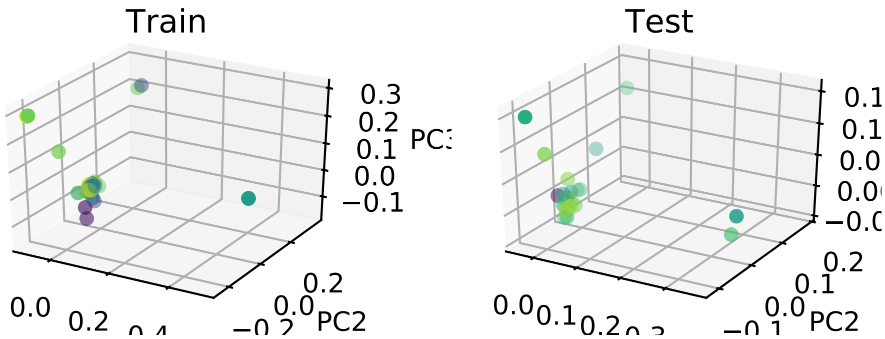
[55]:
```
## create dataframes for training data
df_pca_train = run_pca(matrix_train_tfidf, train_data[['median']], pc=3)
df_pca_train.reset_index(drop=True, inplace=True)

## create dataframes for testing data
df_pca_test = run_pca(matrix_test_tfidf, test_data[['median']], pc=3)
df_pca_test.reset_index(drop=True, inplace=True)

df_pca = pd.concat([df_pca_train, df_pca_test], axis = 0)

df_pca['source'] = ['train']*df_pca_train.shape[0] + ['test']*df_pca_test.
 ↪shape[0]
```

[56]:
```
g = sns.FacetGrid(df_pca, col = 'source', palette = 'seismic');

def facet_scatter(x, y, c, **kwargs):
    kwargs.pop("color")
    plt.scatter(x, y, c=c, **kwargs)

vmin, vmax = 0, 1.2
cmap = plt.cm.viridis

norm=plt.Normalize(vmin=vmin, vmax=vmax)

g = g.map(facet_scatter, 'PC1', 'PC2', 'median',
          s=100, alpha=0.5, norm=norm, cmap=cmap)
```

```
# Make space for the colorbar
g.fig.subplots_adjust(right=.9)

points = plt.scatter([], [], c=[], vmin=vmin, vmax=vmax, cmap=cmap)
g.fig.colorbar(points)

plt.savefig("../images/Fig6c1.png", dpi=410);
plt.show();
```



[57]:
```
fig = plt.figure(figsize=plt.figaspect(0.1))

for i, j in enumerate(['train', 'test']):
    ax = fig.add_subplot(1, len(m_list), i+1, projection='3d')

    ax.set_xlabel('PC1')
    ax.set_ylabel('PC2')
    ax.set_zlabel('PC3')
    ax.set_title(j.capitalize())

    ax.scatter(df_pca.loc[(df_pca.source == j), 'PC1'],
               df_pca.loc[(df_pca.source == j), 'PC2'],
               df_pca.loc[(df_pca.source == j), 'PC3'],
               c=df_pca.loc[(df_pca.source == j), 'median'],
               marker='o',
               cmap=plt.cm.viridis);

plt.savefig("../images/Fig6c2.png", dpi=410);
plt.show();
```



[58]:
```
X_train_tfidf = matrix_train_tfidf
X_train_tfidf['freq'] = list(train_data['Freq'])

X_test_tfidf = matrix_test_tfidf
X_test_tfidf['freq'] = list(test_data['Freq'])
```

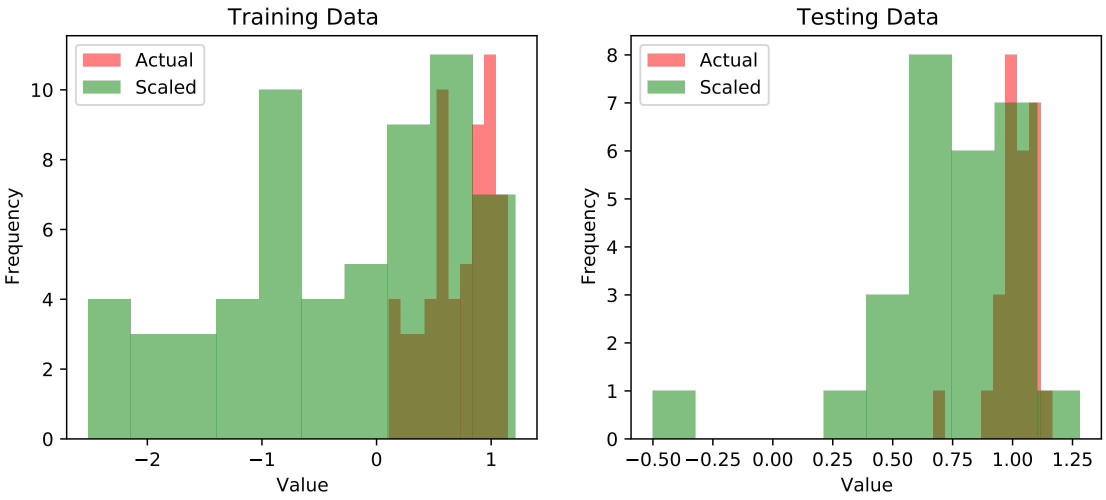
7 Scaling Cell Viability Data

Adapted from here. Not going to scale X values since these are binary variables.

[59]:
```
y_train_unscaled = train_data['median'].to_numpy()
y_test_unscaled = test_data['median'].to_numpy()
```

[60]:
```
sc_y = StandardScaler()

## run standard scaler on all data (including testing) first
y_scaled = merged_data['median'].to_numpy()
y_scaled = sc_y.fit_transform(y_scaled.reshape(-1, 1))

y_train_scaled = y_scaled[merged_data['condition'] != 'pNF']
y_test_scaled = y_scaled[merged_data['condition'] == 'pNF']
```

[61]:
```
fig = plt.figure(figsize = (10,4))
plt.tight_layout()

plt.subplot(1, 2, 1)
plt.hist(train_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_train_scaled, color = 'green', alpha = 0.5);
plt.title('Training Data');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Scaled']);

plt.subplot(1, 2, 2)
plt.hist(test_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_test_scaled, color = 'green', alpha = 0.5);
plt.title('Testing Data');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Scaled']);

plt.savefig("../images/Fig7a.png", dpi=410);
```



8 Linear regression with Lasso regularization

[412]:

```
## set GridSearch and CV parameters

## 5-fold cross-validation on training set
K = 5

## using MSE as score
scorer = make_scorer(mean_squared_error, greater_is_better=False)

## parameters to use for GridSearch
parameters_linreg = [{'alpha': [0, 0.001, 0.01, 0.1, 0.5, 1],
                      'fit_intercept': [True, False],
                      'normalize': [False],
                      'copy_X': [True, False],
                      'max_iter':[100,500,1000,5000],
                      'tol': [1e-5, 1e-4, 1e-3]}]
```

[411]:
```
## run LinReg using GridSearch optimized parameters
def run_lasso(input_x, input_y, params, score, folds):
    lasso_gs = GridSearchCV(linear_model.Lasso(random_state = seed), params,␣
 ↪scoring = score, cv = folds)

    lasso_gs.fit(input_x, input_y)

    print("Best parameters set found on cross-validation:")
    print(lasso_gs.best_params_)

    return lasso_gs
```

8.1 Binary BoW

[413]:
```
random.seed(seed)
np.random.seed(seed)

linreg_bin = run_lasso(X_train_bin,
                       y_train_scaled,
                       params=parameters_linreg,
                       score=scorer,
                       folds=K)
```

```
Best parameters set found on cross-validation:
{'alpha': 0.001, 'copy_X': True, 'fit_intercept': True, 'max_iter': 100,
'normalize': False, 'tol': 1e-05}
```

[414]:
```
#Scaled Data
y_pred_linreg_train_bin = linreg_bin.predict(X_train_bin)
y_pred_linreg_train_bin = sc_y.inverse_transform(y_pred_linreg_train_bin)

y_pred_linreg_test_bin = linreg_bin.predict(X_test_bin)
y_pred_linreg_test_bin = sc_y.inverse_transform(y_pred_linreg_test_bin)

print('Scaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_linreg_train_bin), 6)))
print('Scaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_linreg_test_bin), 6)))
```

```
Scaled training MSE: 0.004461
Scaled test MSE: 0.086494
```

8.2 Count BoW

[415]:

```
linreg_count = run_lasso(X_train_count,
                         y_train_scaled,
                         params=parameters_linreg,
                         score=scorer,
                         folds=K)
```

```
Best parameters set found on cross-validation:
{'alpha': 0.001, 'copy_X': True, 'fit_intercept': True, 'max_iter': 100,
'normalize': False, 'tol': 1e-05}
```

[416]:

```
#Scaled Data
y_pred_linreg_train_count = linreg_count.predict(X_train_count)
y_pred_linreg_train_count = sc_y.inverse_transform(y_pred_linreg_train_count)

y_pred_linreg_test_count = linreg_count.predict(X_test_count)
y_pred_linreg_test_count = sc_y.inverse_transform(y_pred_linreg_test_count)

print('Scaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_linreg_train_count), 6)))
print('Scaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_linreg_test_count), 6)))
```

```
Scaled training MSE: 0.004429
Scaled test MSE: 0.168739
```

8.3 TF-IDF Matrix

[417]:

```
linreg_tfidf = run_lasso(X_train_tfidf,
                         y_train_scaled,
                         params=parameters_linreg,
                         score=scorer,
                         folds=K)
```

```
Best parameters set found on cross-validation:
{'alpha': 0.001, 'copy_X': True, 'fit_intercept': False, 'max_iter': 1000,
'normalize': False, 'tol': 1e-05}
```

[418]:

```
#Scaled Data
y_pred_linreg_train_tfidf = linreg_tfidf.predict(X_train_tfidf)
y_pred_linreg_train_tfidf = sc_y.inverse_transform(y_pred_linreg_train_tfidf)

y_pred_linreg_test_tfidf = linreg_tfidf.predict(X_test_tfidf)
y_pred_linreg_test_tfidf = sc_y.inverse_transform(y_pred_linreg_test_tfidf)
```

```
print('Scaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_linreg_train_tfidf), 6)))
print('Scaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_linreg_test_tfidf), 6)))
```

```
Scaled training MSE: 0.013709
Scaled test MSE: 0.123416
```

8.4 Feature importance inference

[430]:

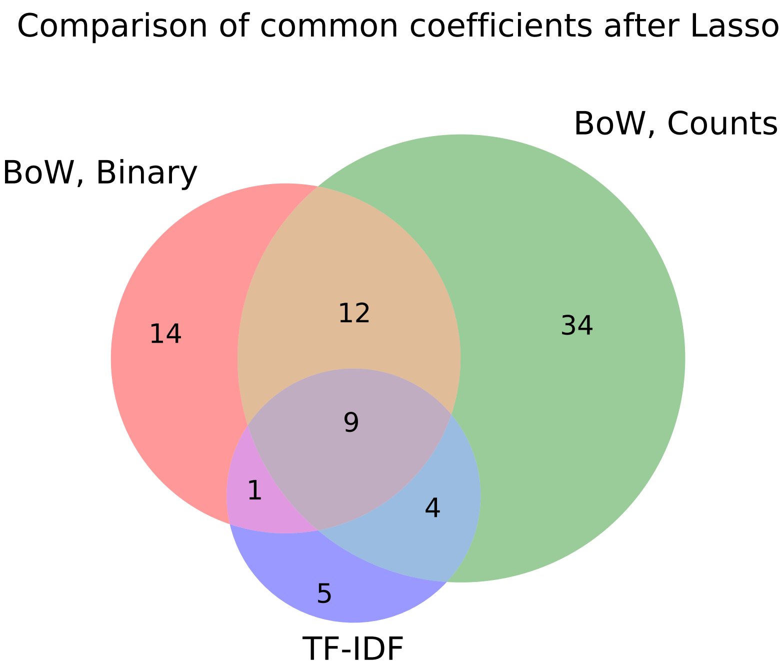
```
def find_coefs(X_input, y_input):

    lasso_model = linear_model.Lasso(alpha=0.001, max_iter=100,
                                     fit_intercept=False,
                                     tol=1e-05, random_state = seed)

    lasso_model.fit(X_input, y_input)

    feature_list = list(X_input.columns)
    coef_list = list(lasso_model.coef_)

    feature_list = [feature_list[i] for i, j in enumerate(coef_list) if j > 0]
    coef_list = [i for i in coef_list if i > 0]

    return coef_list, feature_list
```

[435]:

```
coef_bin, feature_bin = find_coefs(X_train_bin, y_train_scaled)
coef_count, feature_count = find_coefs(X_train_count, y_train_scaled)
coef_tfidf, feature_tfidf = find_coefs(X_train_tfidf, y_train_scaled)

df1 = pd.DataFrame({'features': feature_bin, 'coef_bin': coef_bin})
df2 = pd.DataFrame({'features': feature_count, 'coef_count': coef_count})
df3 = pd.DataFrame({'features': feature_tfidf, 'coef_tfidf': coef_tfidf})

df_coef = pd.merge(df1, df2, on = 'features', how = 'outer')
df_coef = pd.merge(df_coef, df3, on = 'features', how = 'outer')

# df_coef.to_csv('../assets/coefficients.csv', index=False)
```

[419]:

```
venn3([set(feature_bin), set(feature_count), set(feature_tfidf)],
      set_labels = ('BoW, Binary', 'BoW, Counts', 'TF-IDF'));

plt.title('Comparison of common coefficients after Lasso\n');
plt.savefig("../images/Fig8.png", dpi=410);
```



9 SVM Model

Adapted from here.

[62]:
```
## parameters to use for GridSearch
parameters = [{'kernel': ['linear', 'poly', 'sigmoid', 'rbf'],
               'gamma': ['scale', 'auto', 1e-4, 1e-3, 0.01, 0.1, 0.2, 0.5],
               'C': [1, 10, 100, 1000, 10000]}]
```

[63]:
```
## run SVM using GridSearch optimized parameters
def run_svm(input_x, input_y, params, folds, score, eps = 0.01):
    svr_gs = GridSearchCV(SVR(epsilon = eps), params, cv = folds, scoring =␣
 ↪score)

    svr_gs.fit(input_x, input_y.ravel())

    print("Best parameters set found on cross-validation:")
    print(svr_gs.best_params_)

    return svr_gs
```

[64]:
```
## create dataframe from svr_gs object to compare performance
def create_dfcv(input_df):
    C = []
    gamma = []
    kernel = []

    for n in input_df.cv_results_['params']:
        C.append(n['C'])
        gamma.append(n['gamma'])
        kernel.append(n['kernel'])

    df_gs = pd.DataFrame({'C': C, 'gamma': gamma, 'kernel': kernel,
                          'MSE': input_df.cv_results_['mean_test_score'],
                          'SD': input_df.cv_results_['std_test_score']})

    df_gs.MSE = df_gs.MSE.apply(lambda x: -x)

    return df_gs
```

9.1 Binary BoW Matrix

9.1.1 Scaling cell viability

[65]:

```
random.seed(seed)
np.random.seed(seed)

## run model on scaled data
svr_gs_scaled_bin = run_svm(input_x = X_train_bin,
                            input_y = y_train_scaled,
                            params = parameters,
                            folds = K,
                            score = scorer)
```

```
Best parameters set found on cross-validation:
{'C': 100, 'gamma': 'auto', 'kernel': 'rbf'}
```

[66]:

```
y_pred_scaled_train_bin = svr_gs_scaled_bin.predict(X_train_bin)
y_pred_scaled_train_bin = sc_y.inverse_transform(y_pred_scaled_train_bin)

y_pred_scaled_test_bin = svr_gs_scaled_bin.predict(X_test_bin)
y_pred_scaled_test_bin = sc_y.inverse_transform(y_pred_scaled_test_bin)
```

9.1.2 Not scaling cell viability

[67]:

```
random.seed(seed)
np.random.seed(seed)

## run model on unscaled data
svr_gs_unscaled_bin = run_svm(input_x = X_train_bin,
                              input_y = y_train_unscaled,
                              params = parameters,
                              folds = K,
                              score = scorer)
```

```
Best parameters set found on cross-validation:
{'C': 10, 'gamma': 'auto', 'kernel': 'rbf'}
```

[68]:

```
y_pred_unscaled_train_bin = svr_gs_unscaled_bin.predict(X_train_bin)
y_pred_unscaled_test_bin = svr_gs_unscaled_bin.predict(X_test_bin)
```

9.1.3 Summary of scaled vs. unscaled data

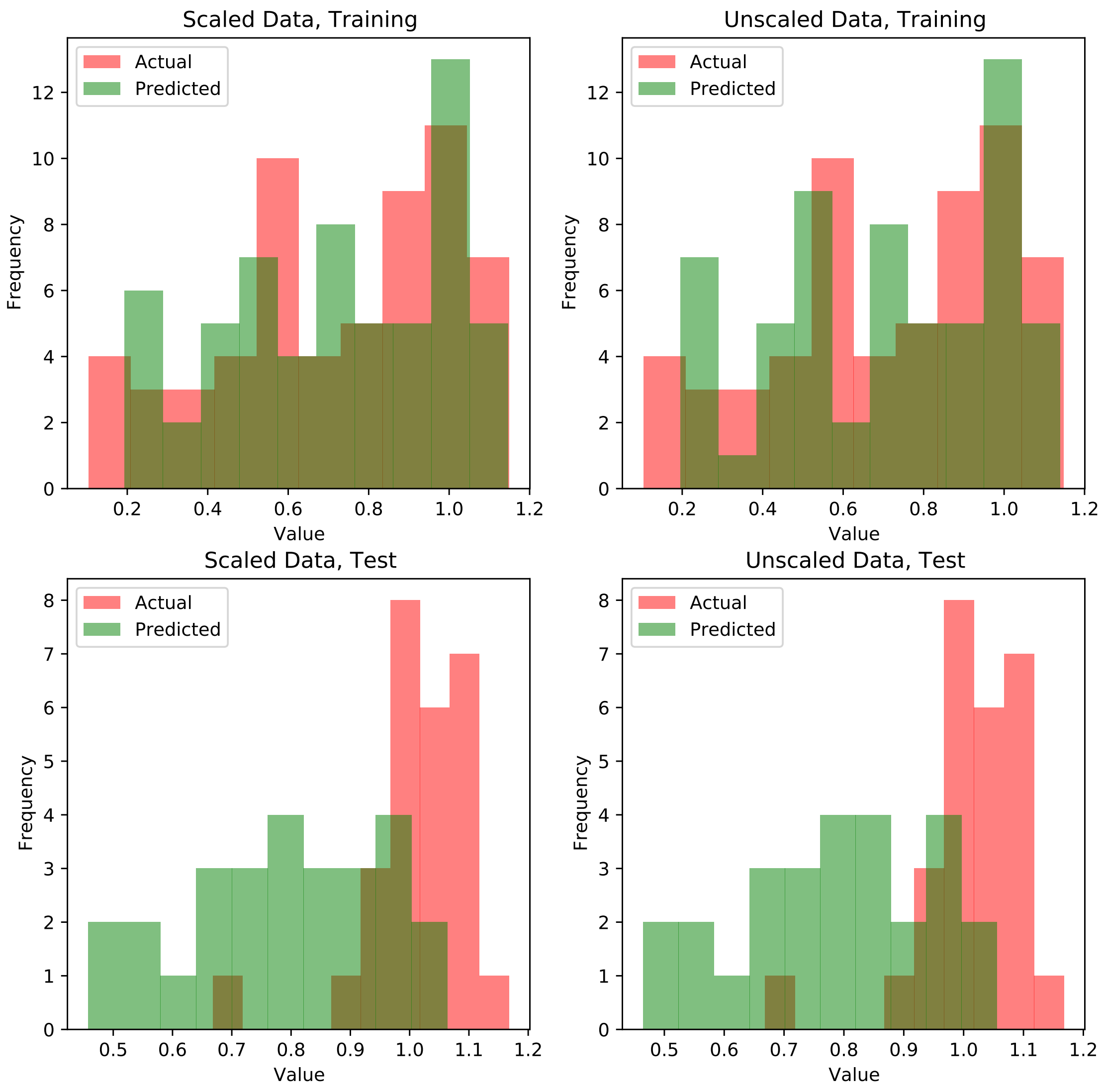
[69]:

```
print('Scaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_scaled_train_bin), 6)))
print('Scaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_scaled_test_bin), 6)))
print()
print('Unscaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_unscaled_train_bin), 6)))
print('Unscaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_unscaled_test_bin), 6)))
```

```
Scaled training MSE: 0.005823
Scaled test MSE: 0.086236

Unscaled training MSE: 0.00577
Unscaled test MSE: 0.085997
```

[70]:

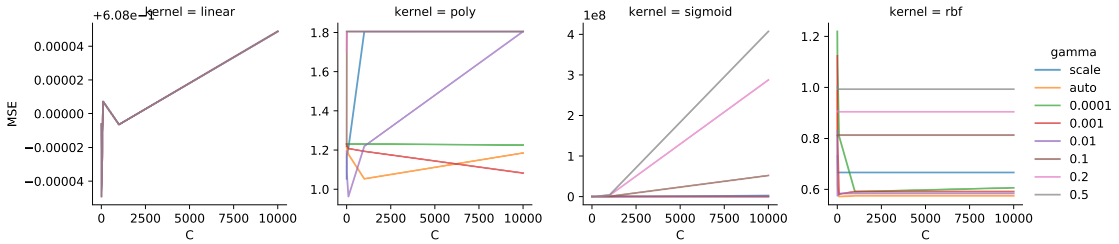
```
fig = plt.figure(figsize = (10,10))
plt.tight_layout()

plt.subplot(2, 2, 1)
plt.hist(train_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_scaled_train_bin, color = 'green', alpha = 0.5);
plt.title('Scaled Data, Training');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 2)
plt.hist(train_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_unscaled_train_bin, color = 'green', alpha = 0.5);
plt.title('Unscaled Data, Training');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 3)
plt.hist(test_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_scaled_test_bin, color = 'green', alpha = 0.5);
plt.title('Scaled Data, Test');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 4)
plt.hist(test_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_unscaled_test_bin, color = 'green', alpha = 0.5);
plt.title('Unscaled Data, Test');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.savefig("../images/Fig7b.png", dpi=410);
```



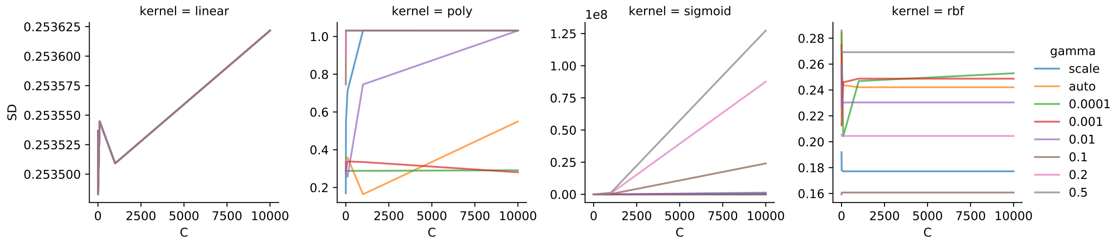
9.1.4 Assessing performance across parameters

[71]:
```
df_gs_svr_bin = create_dfcv(svr_gs_scaled_bin)
```

[72]:
```
g = sns.FacetGrid(df_gs_svr_bin, col = 'kernel', hue = 'gamma', sharey = False);
g.map(sns.lineplot, 'C', 'MSE', alpha=.7);
g.add_legend();
g.savefig("../images/Fig8a.png", bbox_inches = "tight");
```



[73]:
```
g = sns.FacetGrid(df_gs_svr_bin, col = 'kernel', hue = 'gamma', sharey = False);
g.map(sns.lineplot, 'C', 'SD', alpha=.7);
g.add_legend();
g.savefig("../images/Fig8b.png", bbox_inches = "tight");
```



9.2 Count BoW Matrix

9.2.1 Scaling cell viability

[74]:
```
random.seed(seed)
np.random.seed(seed)

## run model on scaled data
svr_gs_scaled_count = run_svm(input_x = X_train_count,
                              input_y = y_train_scaled,
                              params = parameters,
                              folds = K,
                              score = scorer)
```

```
Best parameters set found on cross-validation:
{'C': 100, 'gamma': 'auto', 'kernel': 'rbf'}
```

[75]:
```
y_pred_scaled_train_count = svr_gs_scaled_count.predict(X_train_count)
y_pred_scaled_train_count = sc_y.inverse_transform(y_pred_scaled_train_count)

y_pred_scaled_test_count = svr_gs_scaled_count.predict(X_test_count)
y_pred_scaled_test_count = sc_y.inverse_transform(y_pred_scaled_test_count)
```

9.2.2 Not scaling cell viability

[76]:

```
random.seed(seed)
np.random.seed(seed)

## run model on unscaled data
svr_gs_unscaled_count = run_svm(input_x = X_train_count,
                                input_y = y_train_unscaled,
                                params = parameters,
                                folds = K,
                                score = scorer)
```

```
Best parameters set found on cross-validation:
{'C': 10, 'gamma': 'auto', 'kernel': 'rbf'}
```

[77]:

```
y_pred_unscaled_train_count = svr_gs_unscaled_count.predict(X_train_count)
y_pred_unscaled_test_count = svr_gs_unscaled_count.predict(X_test_count)
```

9.2.3 Summary of scaled vs. unscaled data

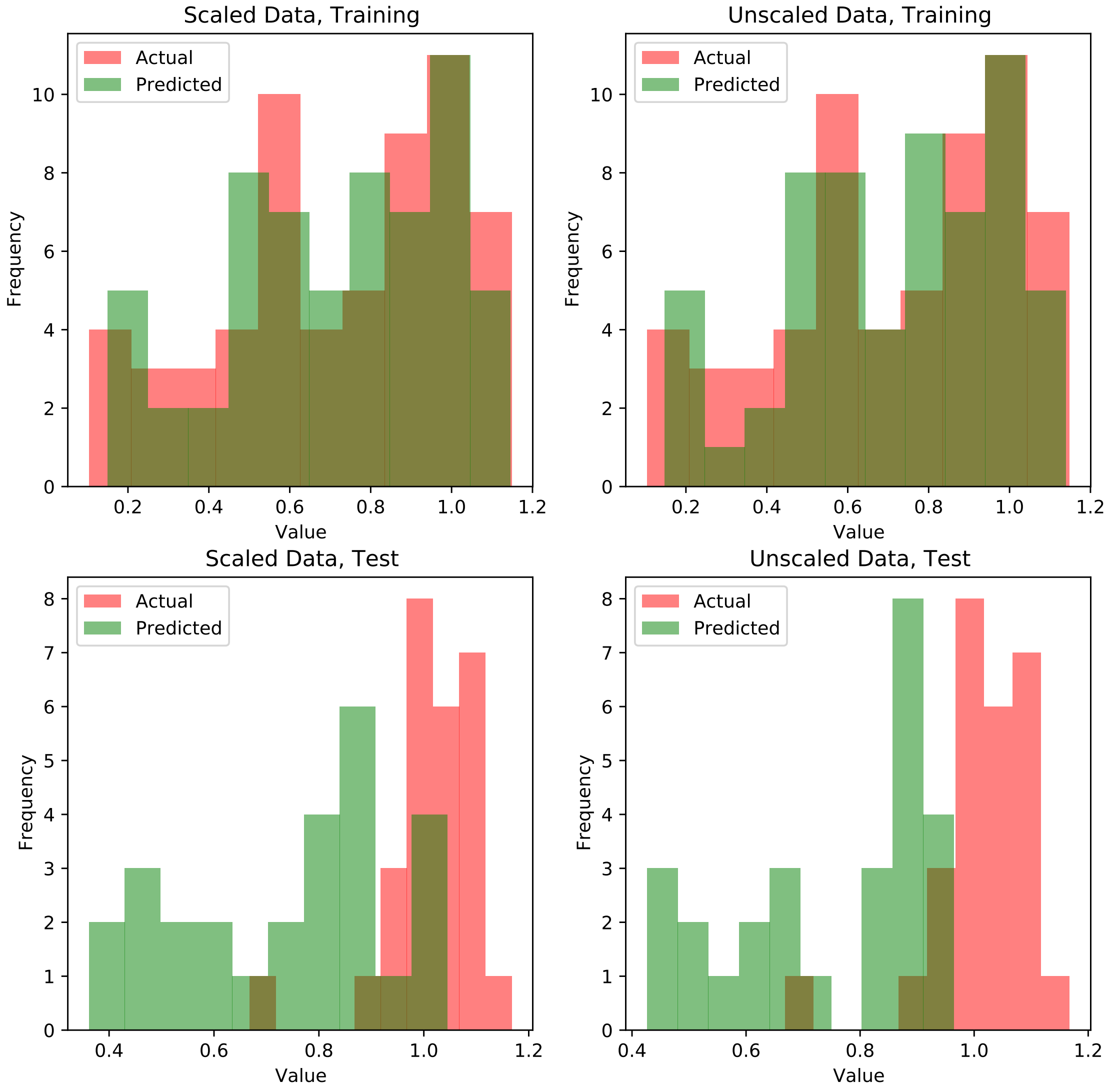
[78]:

```
print('Scaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_scaled_train_count), 6)))
print('Scaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_scaled_test_count), 6)))
print()
print('Unscaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_unscaled_train_count), 6)))
print('Unscaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_unscaled_test_count), 6)))
```

```
Scaled training MSE: 0.005356
Scaled test MSE: 0.117588

Unscaled training MSE: 0.007507
Unscaled test MSE: 0.10732
```

[79]:

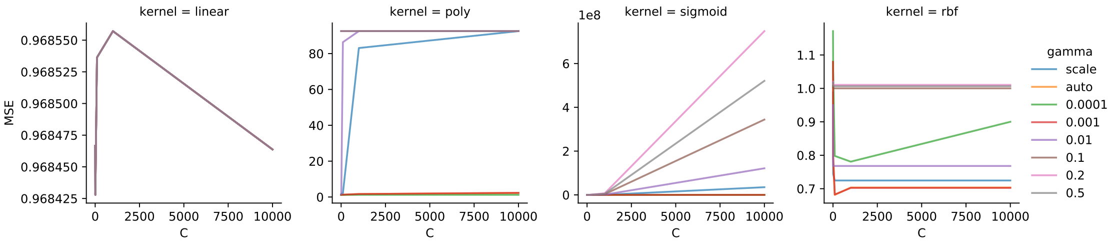
```
fig = plt.figure(figsize = (10,10))
plt.tight_layout()

plt.subplot(2, 2, 1)
plt.hist(train_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_scaled_train_count, color = 'green', alpha = 0.5);
plt.title('Scaled Data, Training');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 2)
plt.hist(train_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_unscaled_train_count, color = 'green', alpha = 0.5);
plt.title('Unscaled Data, Training');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 3)
plt.hist(test_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_scaled_test_count, color = 'green', alpha = 0.5);
plt.title('Scaled Data, Test');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 4)
plt.hist(test_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_unscaled_test_count, color = 'green', alpha = 0.5);
plt.title('Unscaled Data, Test');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.savefig("../images/Fig7b2.png", dpi=410);
```



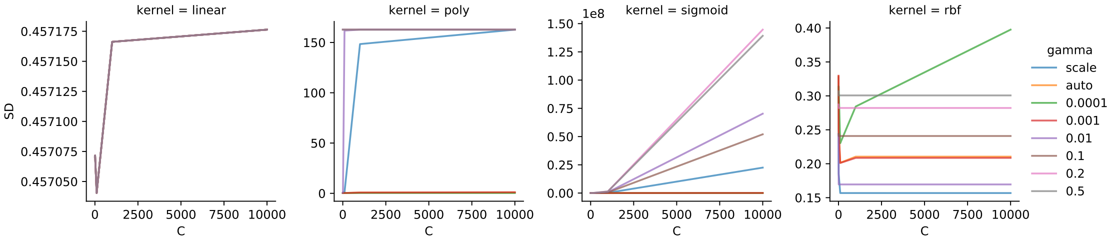
9.2.4 Assessing performance across parameters

```
[80]: df_gs_svr_count = create_dfcv(svr_gs_scaled_count)
```

```
[81]: g = sns.FacetGrid(df_gs_svr_count, col = 'kernel', hue = 'gamma', sharey =␣
       ↪False);
      g.map(sns.lineplot, 'C', 'MSE', alpha=.7);
      g.add_legend();
      g.savefig("../images/Fig8a2.png", bbox_inches = "tight");
```



[82]:
```
g = sns.FacetGrid(df_gs_svr_count, col = 'kernel', hue = 'gamma', sharey =␣
 ↪False);
g.map(sns.lineplot, 'C', 'SD', alpha=.7);
g.add_legend();
g.savefig("../images/Fig8b2.png", bbox_inches = "tight");
```



9.3 TF-IDF Matrix

9.3.1 Scaling cell viability

[83]:
```
random.seed(seed)
np.random.seed(seed)

## run model on scaled data
svr_gs_scaled_tfidf = run_svm(input_x = X_train_tfidf,
                              input_y = y_train_scaled,
                              params = parameters,
                              folds = K,
                              score = scorer)
```

```
Best parameters set found on cross-validation:
{'C': 10000, 'gamma': 0.001, 'kernel': 'sigmoid'}
```

[84]:
```
y_pred_scaled_train_tfidf = svr_gs_scaled_tfidf.predict(X_train_tfidf)
y_pred_scaled_train_tfidf = sc_y.inverse_transform(y_pred_scaled_train_tfidf)

y_pred_scaled_test_tfidf = svr_gs_scaled_tfidf.predict(X_test_tfidf)
y_pred_scaled_test_tfidf = sc_y.inverse_transform(y_pred_scaled_test_tfidf)
```

9.3.2 Not scaling cell viability

[85]:

```
random.seed(seed)
np.random.seed(seed)

## run model on unscaled data
svr_gs_unscaled_tfidf = run_svm(input_x = X_train_tfidf,
                                input_y = y_train_unscaled,
                                params = parameters,
                                folds = K,
                                score = scorer)
```

```
Best parameters set found on cross-validation:
{'C': 10000, 'gamma': 0.0001, 'kernel': 'rbf'}
```

[86]:

```
y_pred_unscaled_train_tfidf = svr_gs_unscaled_tfidf.predict(X_train_tfidf)
y_pred_unscaled_test_tfidf = svr_gs_unscaled_tfidf.predict(X_test_tfidf)
```

9.3.3 Summary of scaled vs. unscaled data

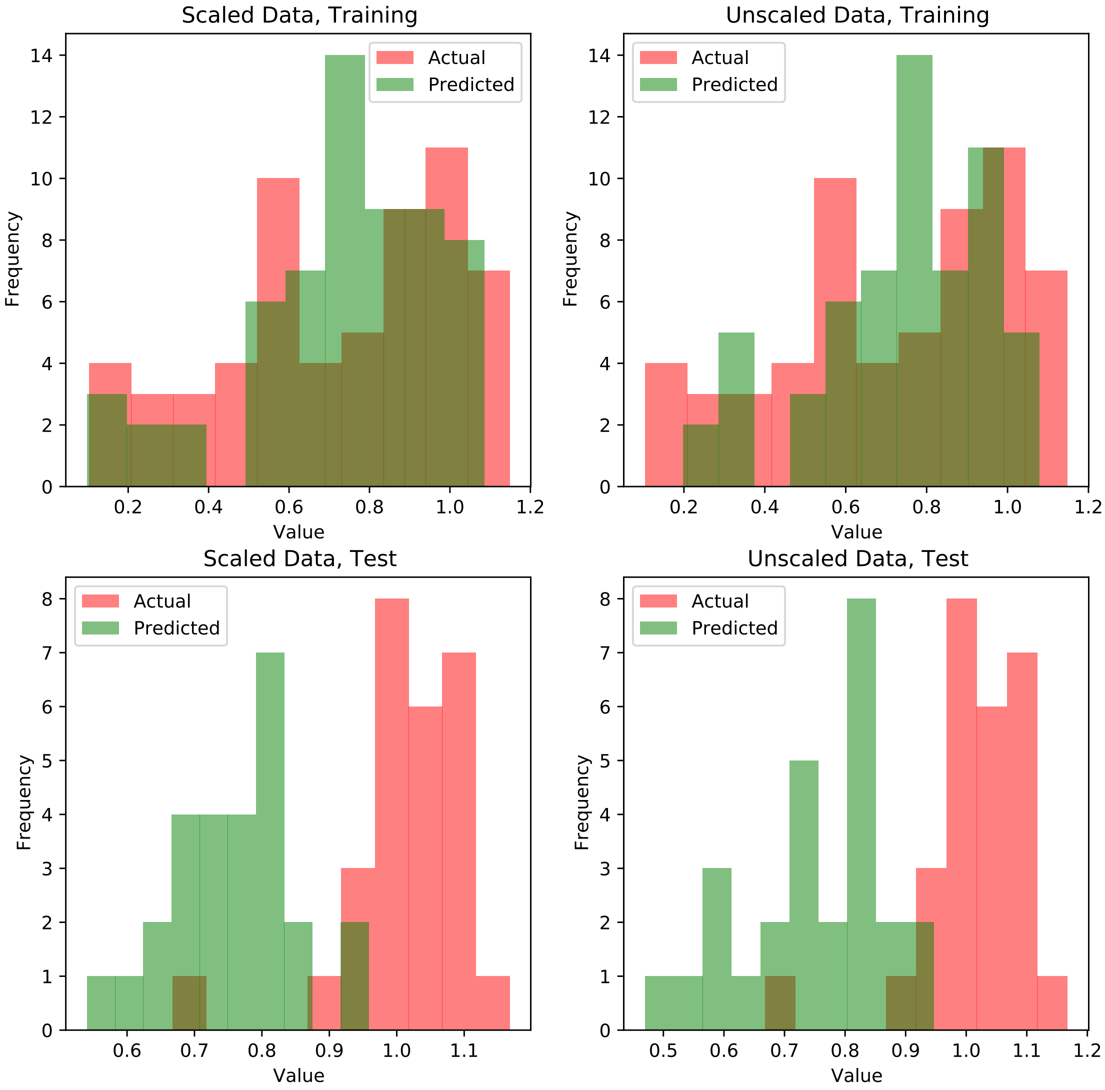
[87]:

```
print('Scaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_scaled_train_tfidf), 6)))
print('Scaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_scaled_test_tfidf), 6)))
print()
print('Unscaled training MSE: {}'.
 ↪format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_unscaled_train_tfidf), 6)))
print('Unscaled test MSE: {}'.
 ↪format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_unscaled_test_tfidf), 6)))
```

```
Scaled training MSE: 0.021364
Scaled test MSE: 0.083281

Unscaled training MSE: 0.025598
Unscaled test MSE: 0.094686
```

[88]:

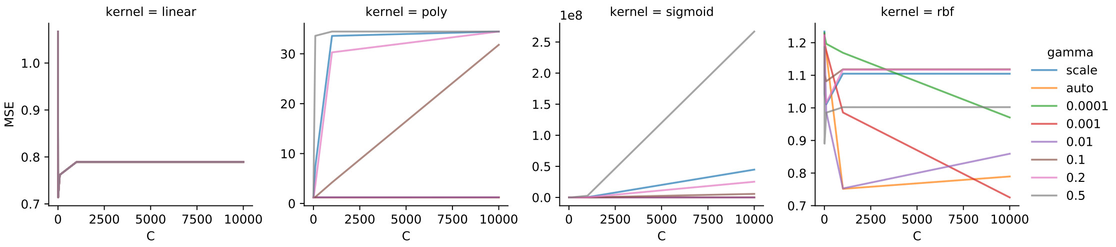
```
fig = plt.figure(figsize = (10,10))
plt.tight_layout()

plt.subplot(2, 2, 1)
plt.hist(train_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_scaled_train_tfidf, color = 'green', alpha = 0.5);
plt.title('Scaled Data, Training');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 2)
plt.hist(train_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_unscaled_train_tfidf, color = 'green', alpha = 0.5);
plt.title('Unscaled Data, Training');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 3)
plt.hist(test_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_scaled_test_tfidf, color = 'green', alpha = 0.5);
plt.title('Scaled Data, Test');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.subplot(2, 2, 4)
plt.hist(test_data['median'], color = 'red', alpha = 0.5);
plt.hist(y_pred_unscaled_test_tfidf, color = 'green', alpha = 0.5);
plt.title('Unscaled Data, Test');
plt.xlabel('Value');
plt.ylabel('Frequency');
plt.legend(labels = ['Actual', 'Predicted']);

plt.savefig("../images/Fig7b3.png", dpi=410);
```



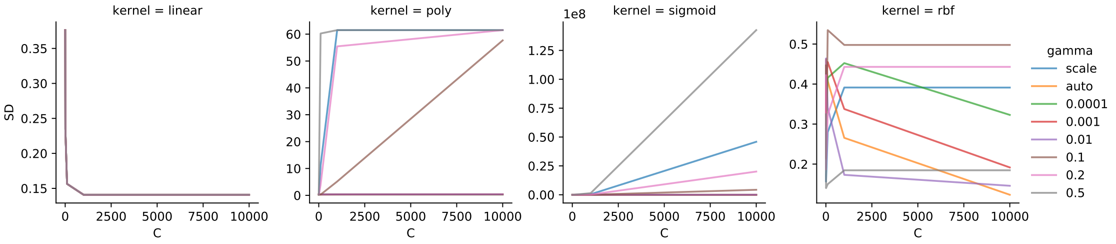
9.3.4 Assessing performance across parameters

[89]:
```
df_gs_svr_tfidf = create_dfcv(svr_gs_scaled_tfidf)
```

[90]:
```
g = sns.FacetGrid(df_gs_svr_tfidf, col = 'kernel', hue = 'gamma', sharey =␣
 ↪False);
g.map(sns.lineplot, 'C', 'MSE', alpha=.7);
g.add_legend();
g.savefig("../images/Fig8a3.png", bbox_inches = "tight");
```



```
[91]: g = sns.FacetGrid(df_gs_svr_tfidf, col = 'kernel', hue = 'gamma', sharey =␣
      ↪False);
      g.map(sns.lineplot, 'C', 'SD', alpha=.7);
      g.add_legend();
      g.savefig("../images/Fig8b3.png", bbox_inches = "tight");
```



10 Gradient Boosting

```
[92]: ## set GridSearch and CV parameters

      ## parameters to use for GridSearch
      parameters = [{'learning_rate': [0.05, 0.1, 0.25, 0.5, 1],
                     'n_estimators': [10, 100, 500, 1000],
                     'subsample': [0.25, 0.50, 0.75, 1.00],
                     'max_depth': [2, 3, 5, 10],
                     'max_features': ['auto', 'sqrt']}]
```

```
[93]: ## run GBM using GridSearch optimized parameters
      def run_gbr(input_x, input_y, params, score, folds):
          gbr_gs = GridSearchCV(GradientBoostingRegressor(random_state=seed), params,␣
      ↪scoring = score, cv = folds)

          gbr_gs.fit(input_x, input_y)

          print("Best parameters set found on cross-validation:")
          print(gbr_gs.best_params_)
```

```
    return gbr_gs
```

[94]:

```
## create dataframe from gbr_gs object to compare performance
def create_dfcv(input_df):
    learning_rate = []
    n_estimators = []
    subsample = []
    max_depth = []
    max_features = []

    for n in input_df.cv_results_['params']:
        learning_rate.append(n['learning_rate'])
        n_estimators.append(n['n_estimators'])
        subsample.append(n['subsample'])
        max_depth.append(n['max_depth'])
        max_features.append(n['max_features'])

    df_gs = pd.DataFrame({'learning_rate': learning_rate,
                          'n_estimators': n_estimators,
                          'subsample': subsample,
                          'max_depth': max_depth,
                          'max_features': max_features,
                          'MSE': input_df.cv_results_['mean_test_score'],
                          'SD': input_df.cv_results_['std_test_score']})

    df_gs.MSE = df_gs.MSE.apply(lambda x: -x)

    return df_gs
```

10.1 Binary BoW Matrix

[95]:

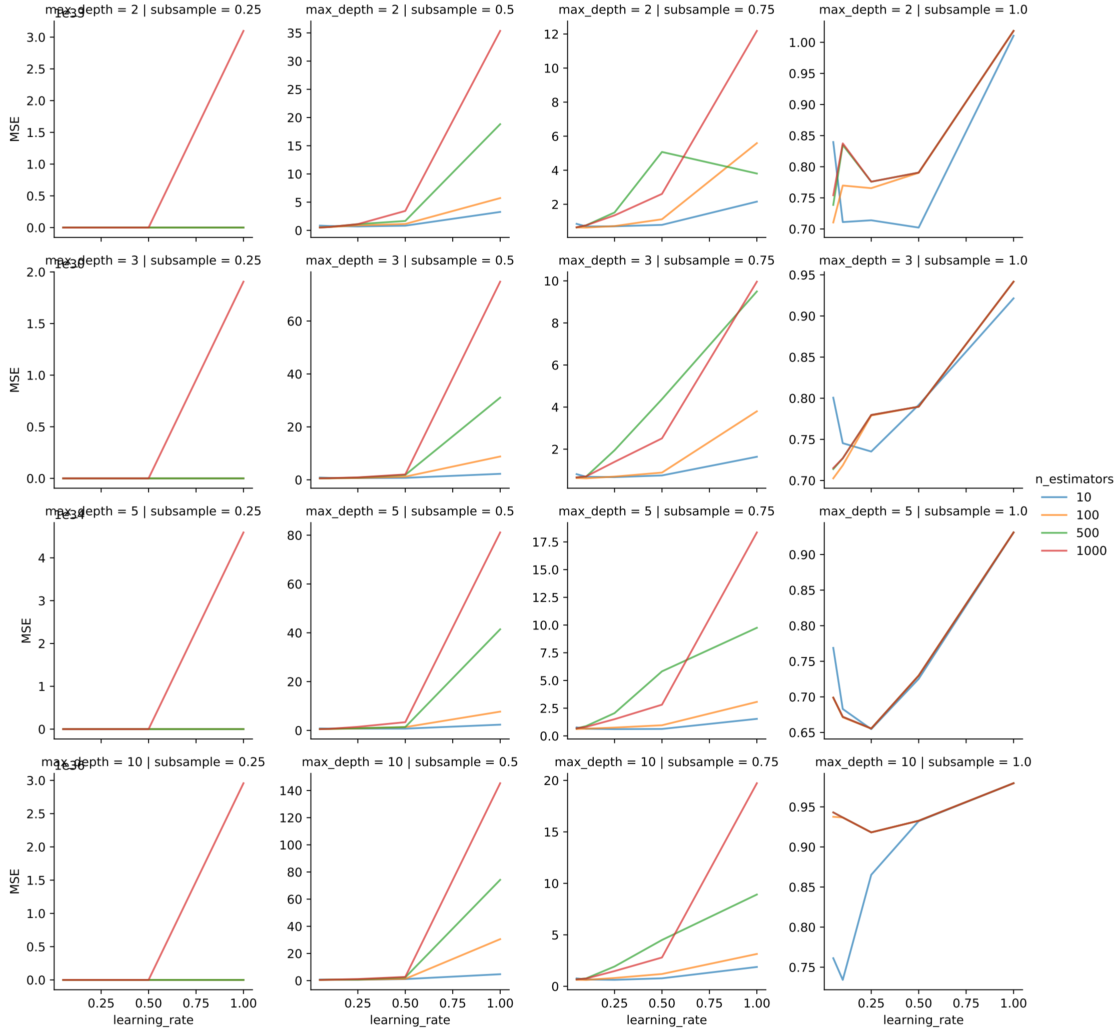
```
random.seed(seed)
np.random.seed(seed)

gbr_bin = run_gbr(matrix_train_bin,
                  y_train_scaled,
                  params=parameters,
                  score=scorer,
                  folds=K)
```

```
Best parameters set found on cross-validation:
{'learning_rate': 0.05, 'max_depth': 2, 'max_features': 'auto', 'n_estimators':
1000, 'subsample': 0.5}
```

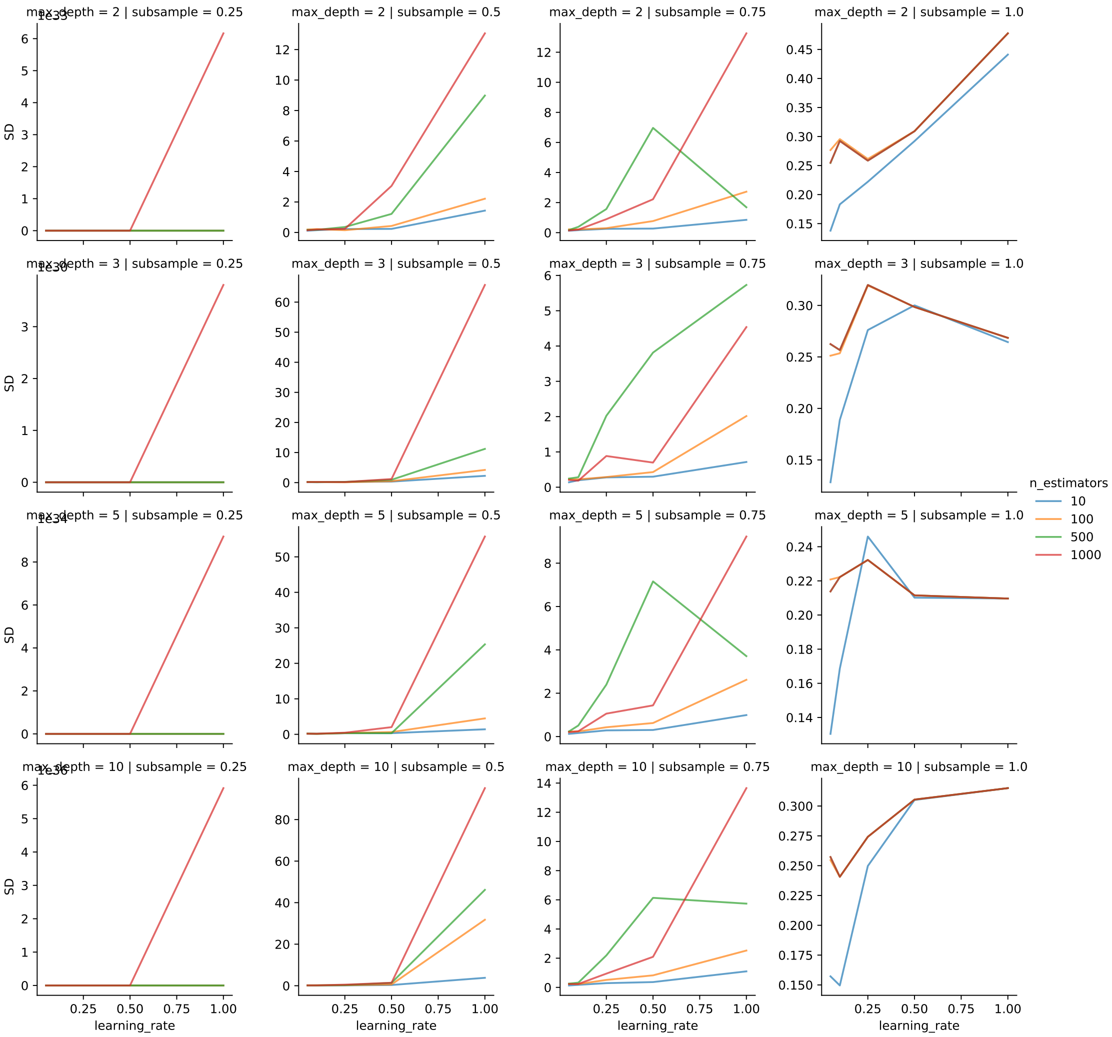
[96]:

```
df_gs_gbr_bin = create_dfcv(gbr_bin)
```

[97]:
```
g = sns.FacetGrid(df_gs_gbr_bin.loc[(df_gs_gbr_bin.max_features == 'auto')],
                  row = 'max_depth', col = 'subsample',
                  hue = 'n_estimators', sharey = False);
g.map(sns.lineplot, 'learning_rate', 'MSE', alpha=.7);
g.add_legend();
g.savefig("../images/Fig11a1.png", bbox_inches = "tight");
```



[98]:
```
g = sns.FacetGrid(df_gs_gbr_bin.loc[(df_gs_gbr_bin.max_features == 'auto')],
                  row = 'max_depth', col = 'subsample',
                  hue = 'n_estimators', sharey = False);
g.map(sns.lineplot, 'learning_rate', 'SD', alpha=.7);
g.add_legend();
g.savefig("../images/Fig11b1.png", bbox_inches = "tight");
```



```
[99]: y_pred_gbr_train_bin = gbr_bin.predict(X_train_bin)
      y_pred_gbr_train_bin = sc_y.inverse_transform(y_pred_gbr_train_bin)

      y_pred_gbr_test_bin = gbr_bin.predict(X_test_bin)
      y_pred_gbr_test_bin = sc_y.inverse_transform(y_pred_gbr_test_bin)
```

```
[100]: print('Training MSE: {}'.format(round(mean_squared_error(train_data['median'],␣
        ↪y_pred_gbr_train_bin), 6)))
       print('Test MSE: {}'.format(round(mean_squared_error(test_data['median'],␣
        ↪y_pred_gbr_test_bin), 6)))
```

```
Training MSE: 0.004813
Test MSE: 0.096419
```

10.2 Count BoW Matrix

[101]:

```
random.seed(seed)
np.random.seed(seed)

gbr_count = run_gbr(matrix_train_count,
                    y_train_scaled,
                    params=parameters,
                    score=scorer,
                    folds=K)
```

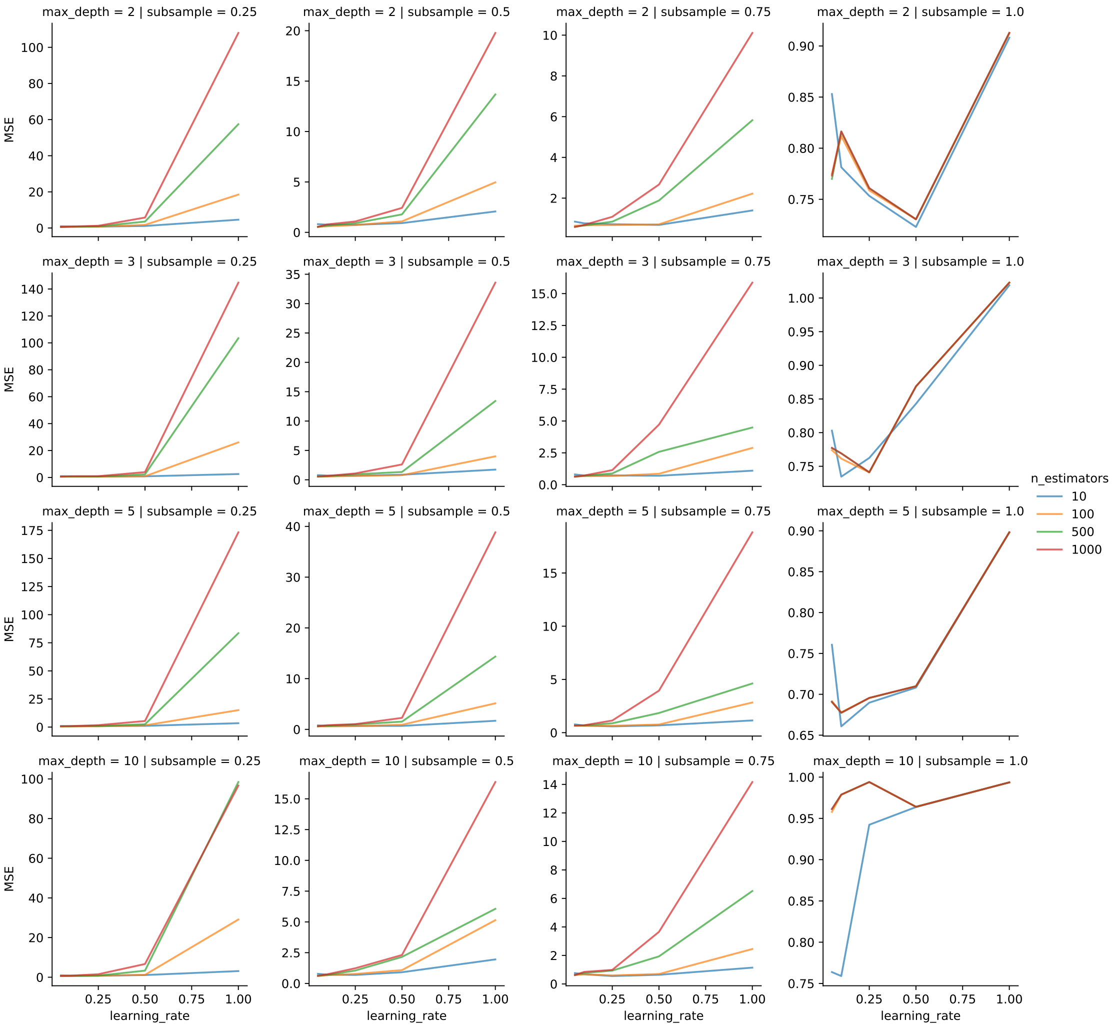
```
Best parameters set found on cross-validation:
{'learning_rate': 0.05, 'max_depth': 3, 'max_features': 'auto', 'n_estimators':
500, 'subsample': 0.5}
```

[102]:

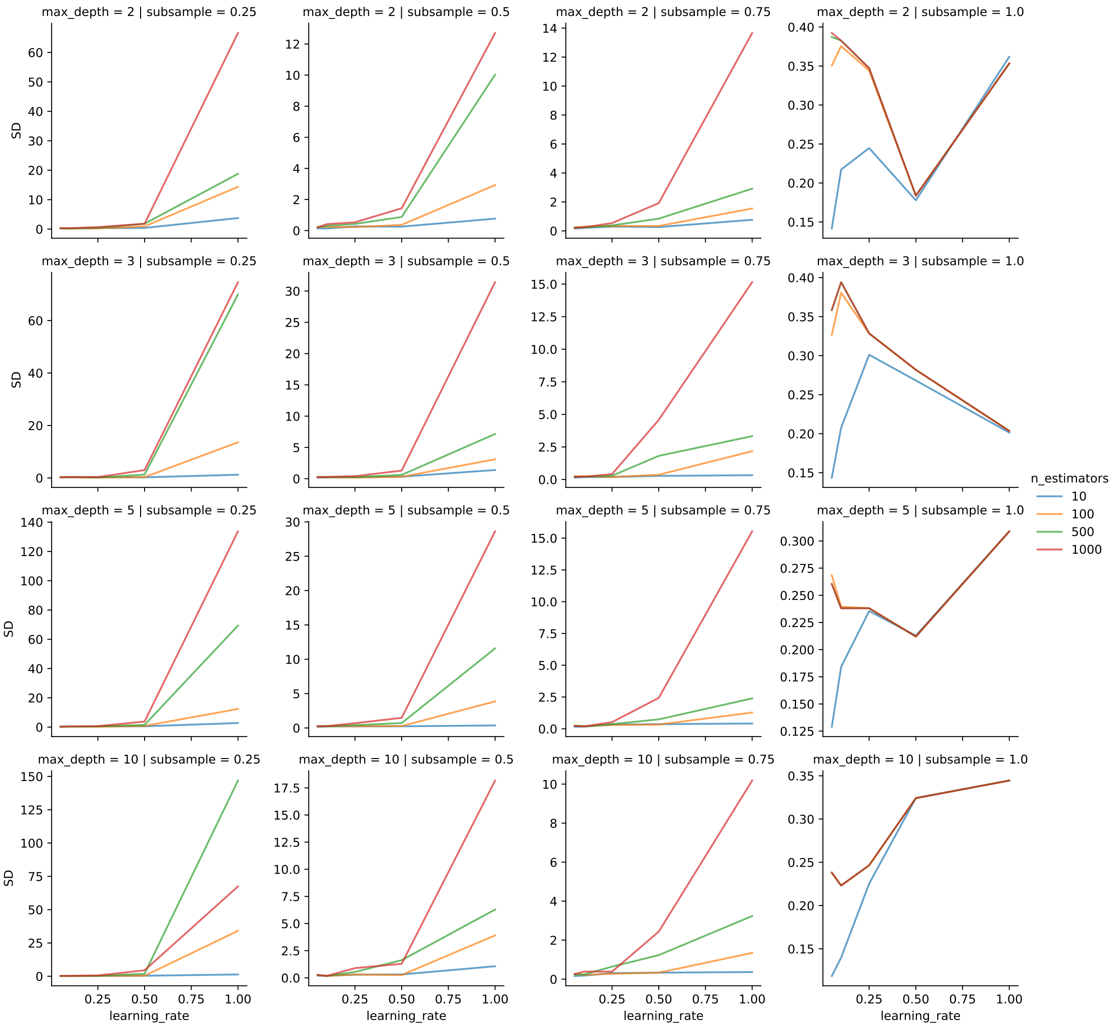
```
df_gs_gbr_count = create_dfcv(gbr_count)
```

[103]:

```
g = sns.FacetGrid(df_gs_gbr_count.loc[(df_gs_gbr_count.max_features == 'auto')],
                  row = 'max_depth', col = 'subsample',
                  hue = 'n_estimators', sharey = False);
g.map(sns.lineplot, 'learning_rate', 'MSE', alpha=.7);
g.add_legend();
g.savefig("../images/Fig11a2.png", bbox_inches = "tight");
```



```
[104]: g = sns.FacetGrid(df_gs_gbr_count.loc[(df_gs_gbr_count.max_features == 'auto')],
                         row = 'max_depth', col = 'subsample',
                         hue = 'n_estimators', sharey = False);
       g.map(sns.lineplot, 'learning_rate', 'SD', alpha=.7);
       g.add_legend();
       g.savefig("../images/Fig11b2.png", bbox_inches = "tight");
```



```
[105]: y_pred_gbr_train_count = gbr_count.predict(X_train_count)
       y_pred_gbr_train_count = sc_y.inverse_transform(y_pred_gbr_train_count)

       y_pred_gbr_test_count = gbr_count.predict(X_test_count)
       y_pred_gbr_test_count = sc_y.inverse_transform(y_pred_gbr_test_count)
```

```
[106]: print('Training MSE: {}'.format(round(mean_squared_error(train_data['median'],␣
        ↪y_pred_gbr_train_count), 6)))
       print('Test MSE: {}'.format(round(mean_squared_error(test_data['median'],␣
        ↪y_pred_gbr_test_count), 6)))
```

```
Training MSE: 0.004714
Test MSE: 0.106614
```

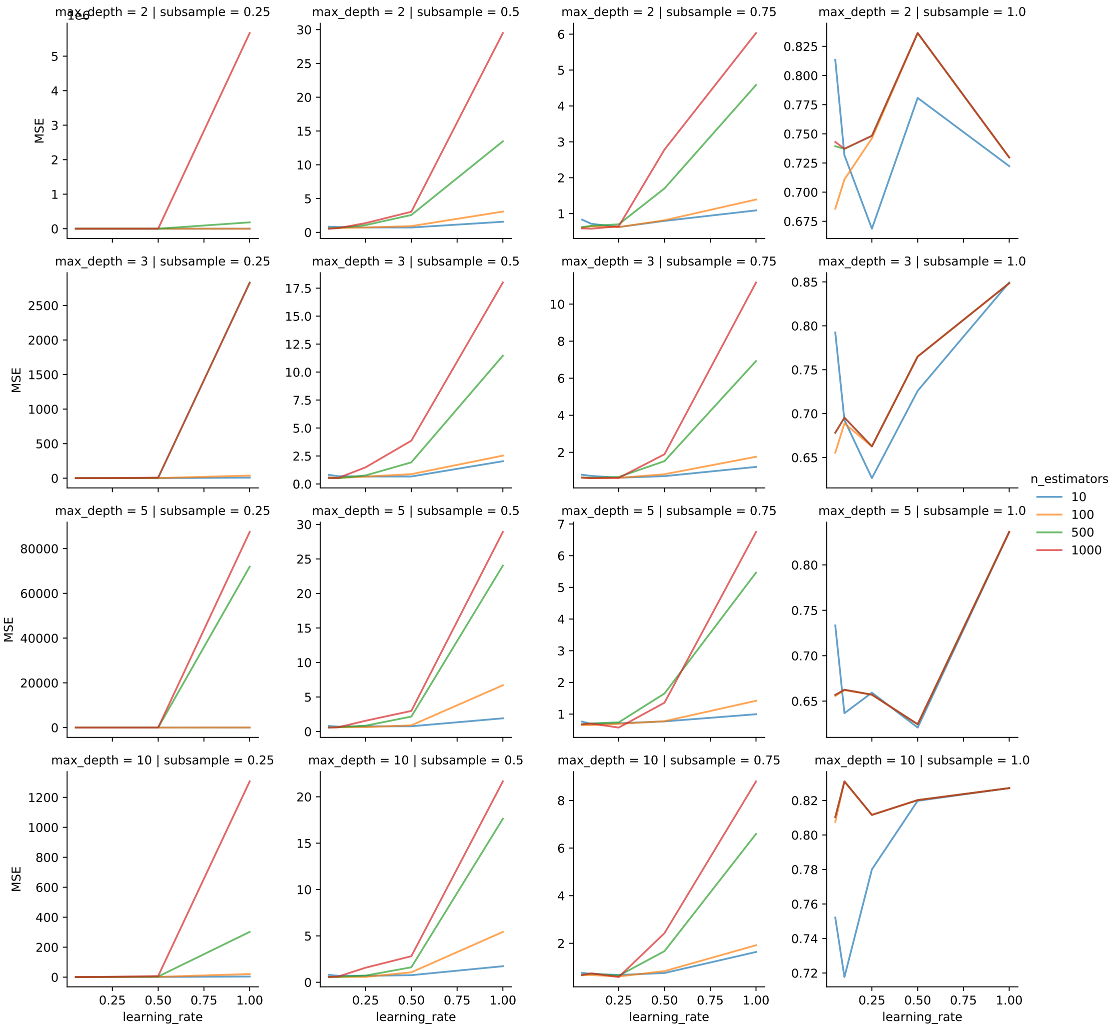
10.3 TF-IDF Matrix

[107]:
```
random.seed(seed)
np.random.seed(seed)

gbr_tfidf = run_gbr(matrix_train_tfidf,
                    y_train_scaled,
                    params=parameters,
                    score=scorer,
                    folds=K)
```

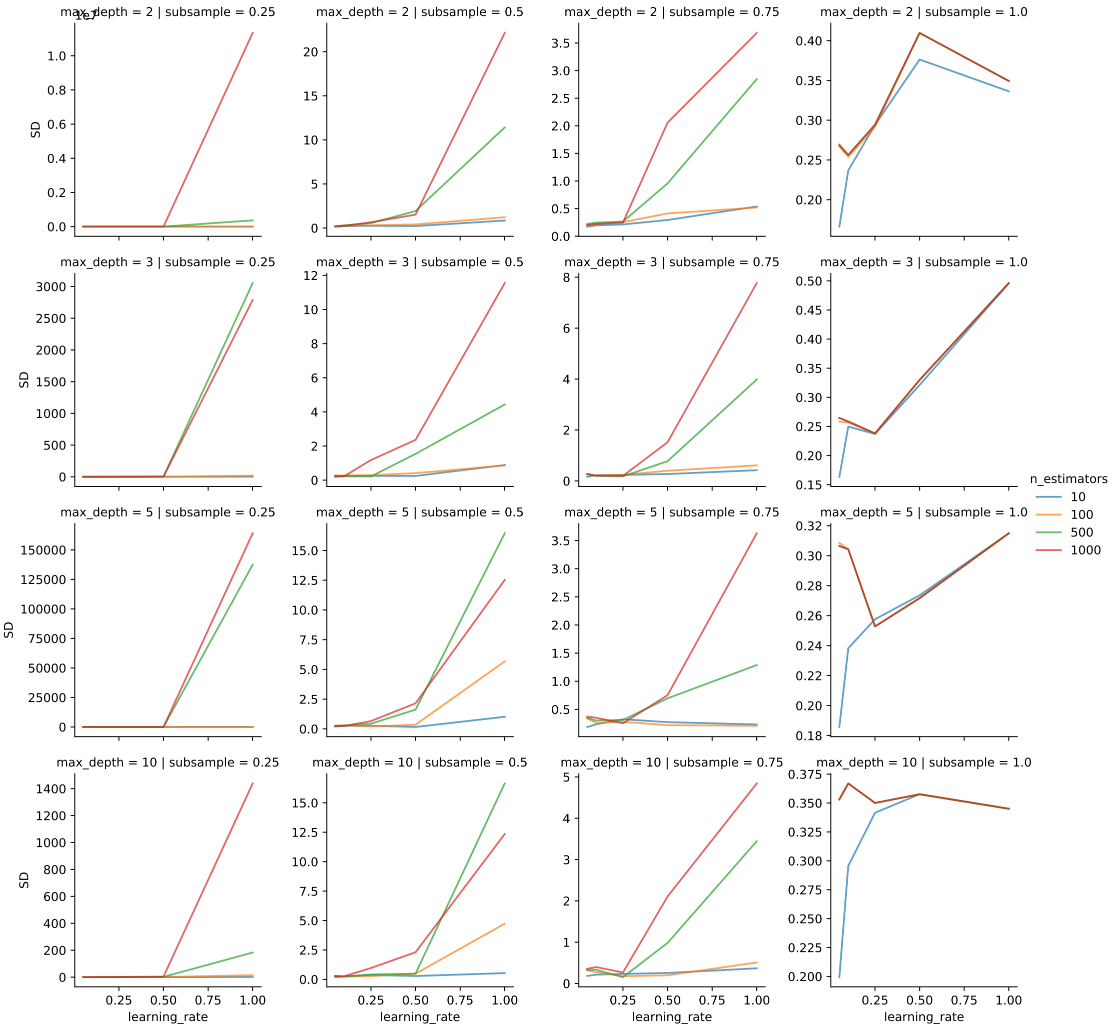
```
Best parameters set found on cross-validation:
{'learning_rate': 0.1, 'max_depth': 3, 'max_features': 'auto', 'n_estimators':
500, 'subsample': 0.5}
```

[108]:
```
df_gs_gbr_tfidif = create_dfcv(gbr_tfidf)
```

[109]:
```
g = sns.FacetGrid(df_gs_gbr_tfidif.loc[(df_gs_gbr_tfidif.max_features ==␣
 ↪'auto')],
                  row = 'max_depth', col = 'subsample',
                  hue = 'n_estimators', sharey = False);
g.map(sns.lineplot, 'learning_rate', 'MSE', alpha=.7);
g.add_legend();
g.savefig("../images/Fig11a3.png", bbox_inches = "tight");
```



```
[110]: g = sns.FacetGrid(df_gs_gbr_tfidif.loc[(df_gs_gbr_tfidif.max_features == 'auto')],
                         row = 'max_depth', col = 'subsample',
                         hue = 'n_estimators', sharey = False);
       g.map(sns.lineplot, 'learning_rate', 'SD', alpha=.7);
       g.add_legend();
       g.savefig("../images/Fig11b3.png", bbox_inches = "tight");
```



[111]:
```
y_pred_gbr_train_tfidf = gbr_tfidf.predict(X_train_tfidf)
y_pred_gbr_train_tfidf = sc_y.inverse_transform(y_pred_gbr_train_tfidf)

y_pred_gbr_test_tfidf = gbr_tfidf.predict(X_test_tfidf)
y_pred_gbr_test_tfidf = sc_y.inverse_transform(y_pred_gbr_test_tfidf)
```

[112]:
```
print('Training MSE: {}'.format(round(mean_squared_error(train_data['median'],␣
 ↪y_pred_gbr_train_tfidf), 6)))
print('Test MSE: {}'.format(round(mean_squared_error(test_data['median'],␣
 ↪y_pred_gbr_test_tfidf), 6)))
```

```
Training MSE: 0.004869
Test MSE: 0.096802
```

11 Compare all methods

```
[436]: df_combo = pd.DataFrame({'Model': ['Lasso']*3 + ['Support Vector']*3 +␣
        ↪['Gradient Boosted']*3,
                                'Matrix': ['BoW, Binary', 'BoW, Count', 'TF-IDF']*3,
                                'MSE_train':␣
        ↪[round(mean_squared_error(train_data['median'], y_pred_linreg_train_bin), 6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_linreg_train_count),␣
        ↪6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_linreg_train_tfidf),␣
        ↪6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_scaled_train_bin), 6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_scaled_train_count),␣
        ↪6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_scaled_train_tfidf),␣
        ↪6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_gbr_train_bin), 6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_gbr_train_count), 6),
                                           ␣
        ↪round(mean_squared_error(train_data['median'], y_pred_gbr_train_tfidf), 6)],
                                'MSE_test':␣
        ↪[round(mean_squared_error(test_data['median'], y_pred_linreg_test_bin), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_linreg_test_count), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_linreg_test_tfidf), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_scaled_test_bin), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_scaled_test_count), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_scaled_test_tfidf), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_gbr_test_bin), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_gbr_test_count), 6),
                                          ␣
        ↪round(mean_squared_error(test_data['median'], y_pred_gbr_test_tfidf), 6)]})
```

[437]:

```
df_combo
```

[437]:

```
              Model       Matrix  MSE_train  MSE_test
0             Lasso  BoW, Binary   0.004461  0.086494
1             Lasso   BoW, Count   0.004429  0.168739
2             Lasso       TF-IDF   0.013709  0.123416
3    Support Vector  BoW, Binary   0.005823  0.086236
4    Support Vector   BoW, Count   0.005356  0.117588
5    Support Vector       TF-IDF   0.021364  0.083281
6  Gradient Boosted  BoW, Binary   0.004813  0.096419
7  Gradient Boosted   BoW, Count   0.004714  0.106614
8  Gradient Boosted       TF-IDF   0.004869  0.096802
```

[224]:

```
def extract_best(input_model, fold):
    keys = list(input_model.best_params_.keys())
    best_param = [input_model.best_params_[k] for k in keys]

    ## create dictionary for grid of parameters
    cv_grid = [list(input_model.cv_results_['param_'+i]) for i in keys]
    dict1 = dict(zip(keys, cv_grid))

    ## create dictionary for CV results by fold
    cv_labels = ['split'+str(i)+'_test_score' for i in range(fold)]
    cv_results = [list(input_model.cv_results_[i]) for i in cv_labels]
    dict2 = dict(zip(cv_labels, cv_results))

    ## combine parameters and CV results into dataframe
    dict1.update(dict2)
    df_cv = pd.DataFrame(dict1)

    ## create list of index where best params occur
    idx_list = [(df_cv[j] == best_param[i]) for i, j in enumerate(keys)]
    idx_lists = [idx for sublist in idx_list for idx, item in␣
 ↪enumerate(sublist) if item == True]

    counter=collections.Counter(idx_lists)

    ## extract location of index where all best parameters occur
    idx = [i for i, j in enumerate(list(counter.values())) if  j == len(keys)]
    idx = list(counter.keys())[idx[0]]

    df_output = df_cv.iloc[[idx]].reset_index(drop=True)

    return df_output
```

[447]:

```
df_1 = extract_best(linreg_bin, K)
df_2 = extract_best(linreg_count, K)
```

```
df_3 = extract_best(linreg_tfidf, K)
df_4 = extract_best(svr_gs_scaled_bin, K)
df_5 = extract_best(svr_gs_scaled_count, K)
df_6 = extract_best(svr_gs_scaled_tfidf, K)
df_7 = extract_best(gbr_bin, K)
df_8 = extract_best(gbr_count, K)
df_9 = extract_best(gbr_tfidf, K)

df_lr = pd.concat([df_1, df_2, df_3])
# df_lr = pd.concat([df_1, df_3])
df_svr = pd.concat([df_4, df_5, df_6])
df_gbr = pd.concat([df_7, df_8, df_9])

col_names = list(df_svr.columns[-K:])
df_cv = pd.concat([df_lr[col_names], df_svr[col_names], df_gbr[col_names]])
df_cv['model'] = ['Lasso']*3 + ['SVR']*3 + ['GBR']*3
# df_cv['model'] = ['LinReg']*2 + ['SVR']*3 + ['GBR']*3
df_cv['source'] = ['BoW, Binary', 'BoW, Count', 'BoW, TF-IDF']*3
# df_cv['source'] = ['BoW, Binary', 'BoW, TF-IDF'] + ['BoW, Binary', 'BoW,␣
 ↪Count', 'BoW, TF-IDF']*2

df_cv = pd.melt(df_cv, id_vars = ['model', 'source'])

df_cv.value = df_cv.value.apply(lambda x: -x)

df_cv['combo'] = df_cv['model'] + '; ' + df_cv['source']

df_cv.sort_values(by='combo', ascending=False, inplace=True)
```

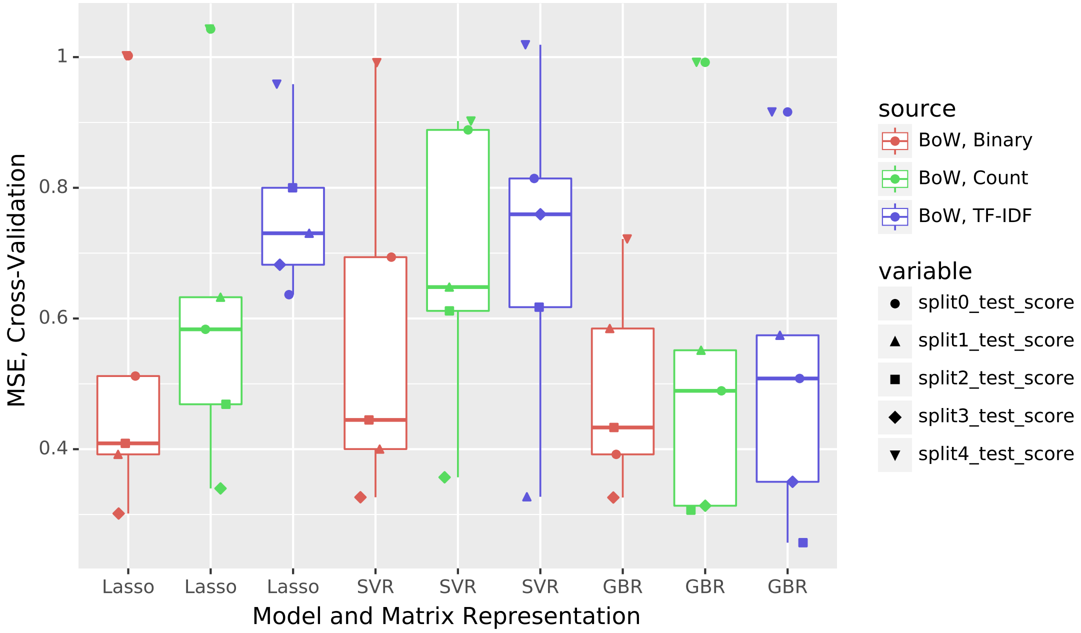
[442]:
```
df_cv
```

[442]:
```
   model       source          variable     value            combo
14   SVR  BoW, TF-IDF  split1_test_score  0.327188  SVR; BoW, TF-IDF
23   SVR  BoW, TF-IDF  split2_test_score  0.617350  SVR; BoW, TF-IDF
32   SVR  BoW, TF-IDF  split3_test_score  0.759470  SVR; BoW, TF-IDF
5    SVR  BoW, TF-IDF  split0_test_score  0.814282  SVR; BoW, TF-IDF
41   SVR  BoW, TF-IDF  split4_test_score  1.018901  SVR; BoW, TF-IDF
22   SVR   BoW, Count  split2_test_score  0.611655   SVR; BoW, Count
31   SVR   BoW, Count  split3_test_score  0.356973   SVR; BoW, Count
13   SVR   BoW, Count  split1_test_score  0.648075   SVR; BoW, Count
4    SVR   BoW, Count  split0_test_score  0.888607   SVR; BoW, Count
40   SVR   BoW, Count  split4_test_score  0.902189   SVR; BoW, Count
30   SVR  BoW, Binary  split3_test_score  0.326434  SVR; BoW, Binary
21   SVR  BoW, Binary  split2_test_score  0.444757  SVR; BoW, Binary
3    SVR  BoW, Binary  split0_test_score  0.693866  SVR; BoW, Binary
39   SVR  BoW, Binary  split4_test_score  0.991545  SVR; BoW, Binary
12   SVR  BoW, Binary  split1_test_score  0.400171  SVR; BoW, Binary
```

```
38  LinReg  BoW, TF-IDF  split4_test_score  0.958578  LinReg; BoW, TF-IDF
20  LinReg  BoW, TF-IDF  split2_test_score  0.800024  LinReg; BoW, TF-IDF
11  LinReg  BoW, TF-IDF  split1_test_score  0.730442  LinReg; BoW, TF-IDF
2   LinReg  BoW, TF-IDF  split0_test_score  0.636475  LinReg; BoW, TF-IDF
29  LinReg  BoW, TF-IDF  split3_test_score  0.682269  LinReg; BoW, TF-IDF
37  LinReg   BoW, Count  split4_test_score  1.042973   LinReg; BoW, Count
19  LinReg   BoW, Count  split2_test_score  0.468739   LinReg; BoW, Count
1   LinReg   BoW, Count  split0_test_score  0.583421   LinReg; BoW, Count
10  LinReg   BoW, Count  split1_test_score  0.632564   LinReg; BoW, Count
28  LinReg   BoW, Count  split3_test_score  0.339919   LinReg; BoW, Count
27  LinReg  BoW, Binary  split3_test_score  0.301539  LinReg; BoW, Binary
36  LinReg  BoW, Binary  split4_test_score  1.002065  LinReg; BoW, Binary
0   LinReg  BoW, Binary  split0_test_score  0.511919  LinReg; BoW, Binary
18  LinReg  BoW, Binary  split2_test_score  0.408925  LinReg; BoW, Binary
9   LinReg  BoW, Binary  split1_test_score  0.392092  LinReg; BoW, Binary
26     GBR  BoW, TF-IDF  split2_test_score  0.256925     GBR; BoW, TF-IDF
35     GBR  BoW, TF-IDF  split3_test_score  0.350075     GBR; BoW, TF-IDF
8      GBR  BoW, TF-IDF  split0_test_score  0.508201     GBR; BoW, TF-IDF
44     GBR  BoW, TF-IDF  split4_test_score  0.916063     GBR; BoW, TF-IDF
17     GBR  BoW, TF-IDF  split1_test_score  0.574304     GBR; BoW, TF-IDF
34     GBR   BoW, Count  split3_test_score  0.313460      GBR; BoW, Count
25     GBR   BoW, Count  split2_test_score  0.306678      GBR; BoW, Count
7      GBR   BoW, Count  split0_test_score  0.489307      GBR; BoW, Count
43     GBR   BoW, Count  split4_test_score  0.992053      GBR; BoW, Count
16     GBR   BoW, Count  split1_test_score  0.551400      GBR; BoW, Count
33     GBR  BoW, Binary  split3_test_score  0.326051     GBR; BoW, Binary
15     GBR  BoW, Binary  split1_test_score  0.584687     GBR; BoW, Binary
24     GBR  BoW, Binary  split2_test_score  0.433207     GBR; BoW, Binary
6      GBR  BoW, Binary  split0_test_score  0.392073     GBR; BoW, Binary
42     GBR  BoW, Binary  split4_test_score  0.721689     GBR; BoW, Binary
```

[448]:

```
from plotnine import ggplot, aes, geom_boxplot, geom_jitter, position_jitter, \
    theme, element_text, xlab, ylab, scale_x_discrete

lab_list = ['Lasso; BoW, Binary', 'Lasso; BoW, Count', 'Lasso; BoW, TF-IDF',
            'SVR; BoW, Binary', 'SVR; BoW, Count', 'SVR; BoW, TF-IDF',
            'GBR; BoW, Binary', 'GBR; BoW, Count', 'GBR; BoW, TF-IDF']

labs = ['Lasso']*3 + ['SVR']*3 + ['GBR']*3

(
    ggplot(df_cv)  # What data to use
    + geom_boxplot(mapping=aes(x='combo', y='value', color='source'))
    + geom_jitter(mapping=aes(x='combo', y='value', color='source',␣
 ↪shape='variable'),
                  position=position_jitter(0.2))
    + xlab('Model and Matrix Representation')
    + ylab('MSE, Cross-Validation')
    + scale_x_discrete(labels = labs,
                       limits=lab_list)
)
```



```
[448]: <ggplot: (110188265391)>
```

12 Assessing Model Performance on Test Data

[468]:
```
n_test = test_data.shape[0]

bin_list = list(y_pred_linreg_test_bin.reshape(n_test)) +␣
 ↪list(y_pred_scaled_test_bin) + list(y_pred_gbr_test_bin)
count_list = list(y_pred_linreg_test_count.reshape(n_test)) +␣
 ↪list(y_pred_scaled_test_count) + list(y_pred_gbr_test_count)
tfidf_list = list(y_pred_linreg_test_tfidf.reshape(n_test)) +␣
 ↪list(y_pred_scaled_test_tfidf) + list(y_pred_gbr_test_tfidf)
```

[469]:
```
df_pred = pd.DataFrame({'drug': list(test_data.drug)*3,
                        'y_pred_bin': bin_list,
                        'y_pred_count': count_list,
                        'y_pred_tfidf': tfidf_list,
                        'model': ['Lasso']*n_test + ['SVR']*n_test +␣
 ↪['GBR']*n_test,
                        'y_actual': list(test_data['median'])*3})
df_pred.reset_index(drop=True, inplace=True)
```

[470]:
```
## manually replace those with naming mismatches
df_moa.Drugs[df_moa.Drugs == 'mycophenolatemofetil'] = 'mycophenolate mofetil'
df_moa.Drugs[df_moa.Drugs == 'tamoxifen citrate'] = 'tamoxifen'
df_moa.Drugs[df_moa.Drugs == 'ketotifen fumarate'] = 'ketotifen'
df_moa.Drugs[df_moa.Drugs == 'minocycline hydrochloride'] = 'minocycline'
df_moa.Drugs[df_moa.Drugs == 'tetracycline hydrochloride'] = 'tetracycline'
df_moa.Drugs[df_moa.Drugs == 'trifluoperazine dihydrochloride'] =␣
 ↪'trifluoperazine'
```

[471]:
```
df_pred = df_pred.merge(df_moa.loc[:, ['Drugs', 'moa_final']],
                        left_on='drug', right_on='Drugs', how='inner')
```

[472]:
```
df_pred.loc[(df_pred.drug == 'octreotide'), 'moa_final'] = 'somatostatin␣
 ↪analogue'
df_pred.loc[(df_pred.drug == 'tipifarnib'), 'moa_final'] = 'farnesyltransferase␣
 ↪inhibitor'
```

[473]:
```
df_pred.drop(columns='Drugs', inplace=True)
```

[474]:
```
## take the first MOA listed
df_pred['moa_final'] = df_pred['moa_final'].apply(lambda x: x.split(',')[0])
```

[475]:
```
df_pred.moa_final.value_counts()/3
```

[475]:
```
MEK inhibitor                                4.0
bacterial 30S ribosomal subunit inhibitor    3.0
FLT3 inhibitor                               2.0
mTOR inhibitor                               2.0
progesterone receptor agonist                1.0
estrogen receptor antagonist                 1.0
estrogen receptor agonist                    1.0
cyclooxygenase inhibitor                     1.0
histamine receptor agonist                   1.0
Abl kinase inhibitor                         1.0
Bcr-Abl kinase inhibitor                     1.0
androgen receptor agonist                    1.0
HMGCR inhibitor                              1.0
dopamine receptor antagonist                 1.0
tubulin polymerization inhibitor             1.0
topoisomerase inhibitor                      1.0
dehydrogenase inhibitor                      1.0
calcineurin inhibitor                        1.0
Name: moa_final, dtype: float64
```

AdjustTexts adapted from here and here.

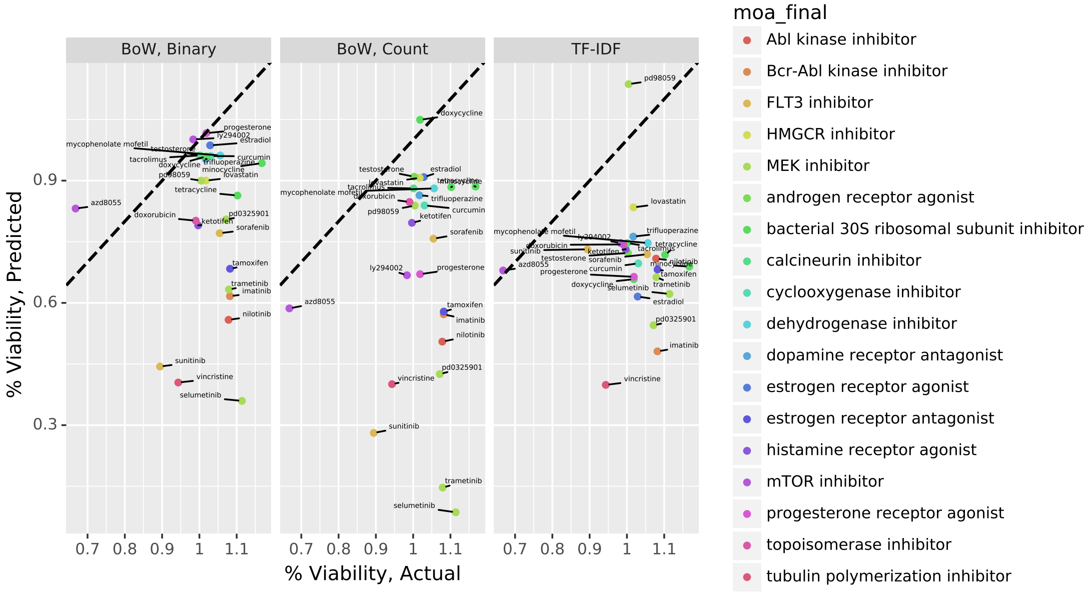
[476]:

```
df_pred = pd.melt(df_pred, id_vars = ['drug', 'y_actual', 'moa_final', 'model'])

df_pred['delta'] = df_pred['y_actual'] - df_pred['value']

df_pred.sort_values(by='delta', ascending=False, inplace=True)

df_pred.variable.loc[(df_pred.variable == 'y_pred_bin')] = 'BoW, Binary'
df_pred.variable.loc[(df_pred.variable == 'y_pred_count')] = 'BoW, Count'
df_pred.variable.loc[(df_pred.variable == 'y_pred_tfidf')] = 'TF-IDF'
```

Adjust text dictionary adopted from here.

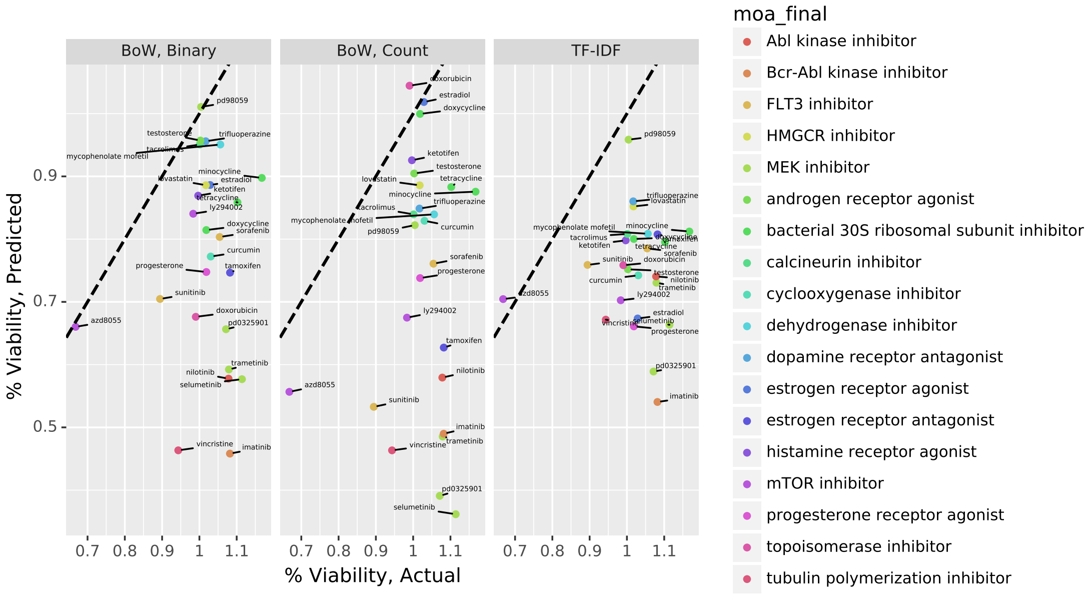
[458]:

```
from plotnine import ggplot, aes, geom_point, facet_grid, geom_abline,␣
 ↪geom_text, xlab, ylab

adjust_text_dict = {
    'expand_points': (2, 2),
    'arrowprops': {
        'arrowstyle': '-',
        'color': 'black'
    }
}

(
    ggplot(df_pred.loc[df_pred.model == 'Lasso'])  # What data to use
    + geom_point(mapping=aes(x='y_actual', y='value', color='moa_final'))  #␣
 ↪What variable to use
    + facet_wrap('~variable')  # Geometric object to use for drawing
    + geom_abline(intercept = 0, slope = 1, linetype="dashed", size=1)
    + geom_text(mapping=aes(x='y_actual', y='value', label='drug'),
                nudge_x = 0.1, nudge_y = 0.1, size=4, adjust_text =␣
 ↪adjust_text_dict)
    + xlab('% Viability, Actual')
    + ylab('% Viability, Predicted')
)
```



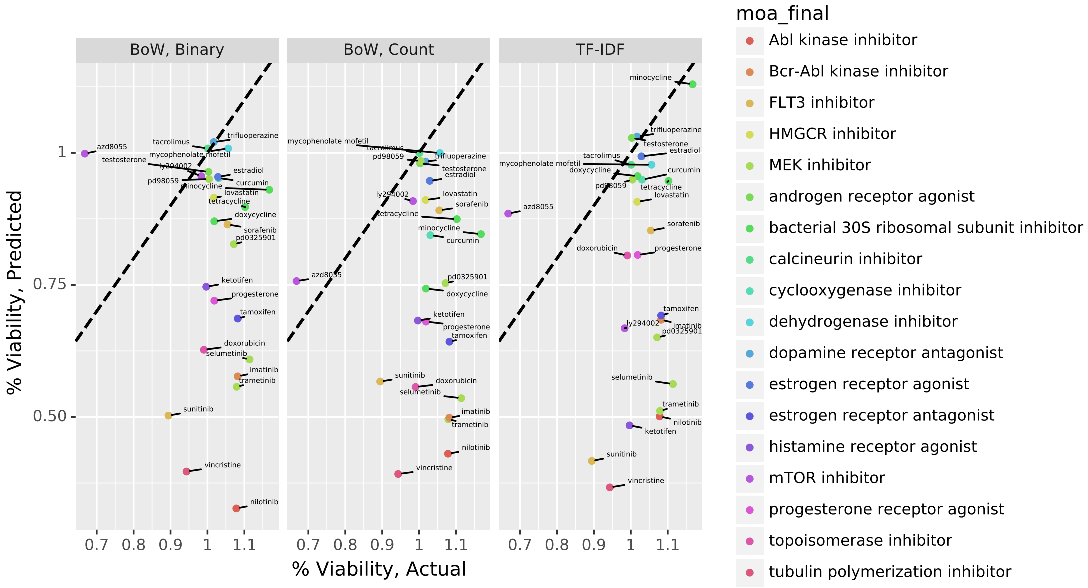
```
[458]: <ggplot: (110189456267)>
```

```
[374]: from plotnine import ggplot, aes, geom_point, facet_grid, geom_abline,␣
        ↪geom_text, xlab, ylab

       adjust_text_dict = {
           'expand_points': (2, 2),
           'arrowprops': {
               'arrowstyle': '-',
               'color': 'black'
           }
       }

       (
           ggplot(df_pred.loc[df_pred.model == 'SVR'])  # What data to use
           + geom_point(mapping=aes(x='y_actual', y='value', color='moa_final'))  #␣
        ↪What variable to use
           + facet_wrap('~variable')  # Geometric object to use for drawing
           + geom_abline(intercept = 0, slope = 1, linetype="dashed", size=1)
           + geom_text(mapping=aes(x='y_actual', y='value', label='drug'),
                       nudge_x = 0.1, nudge_y = 0.1, size=4, adjust_text =␣
        ↪adjust_text_dict)
           + xlab('% Viability, Actual')
           + ylab('% Viability, Predicted')
       )
```



[374]: <ggplot: (110059480188)>

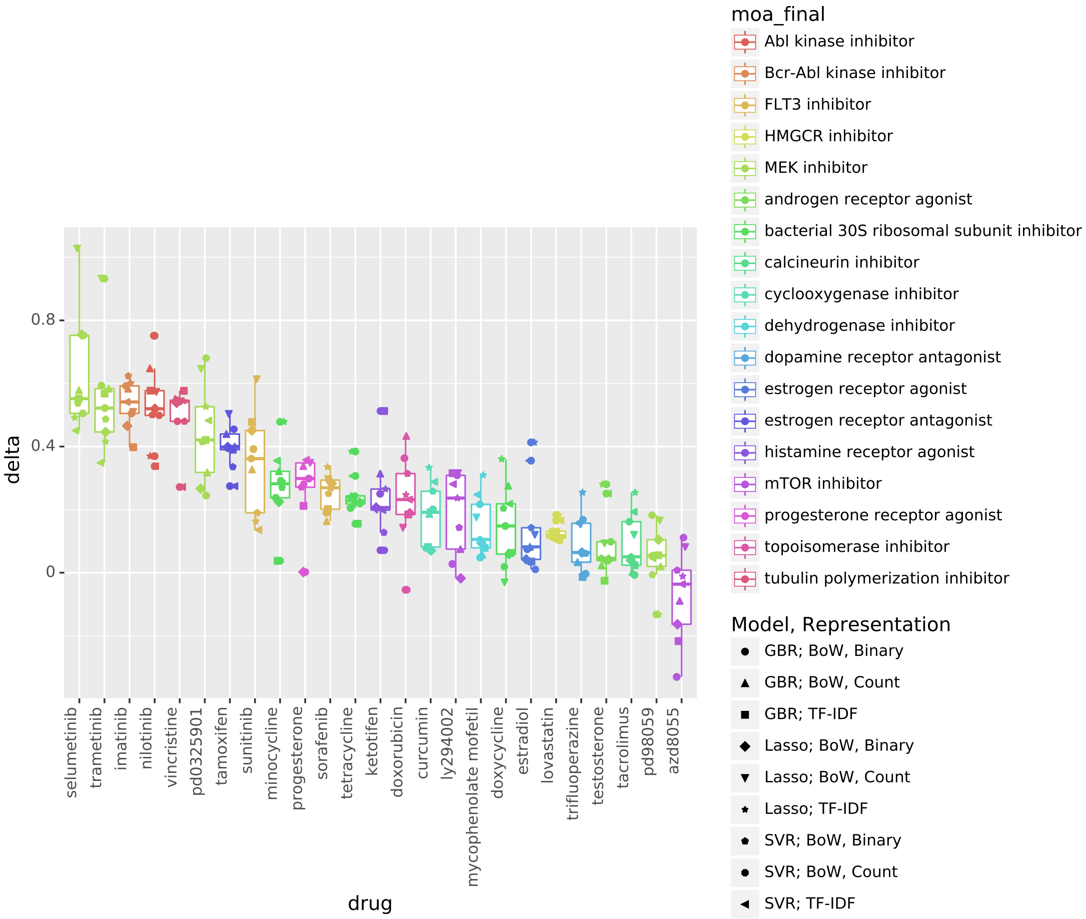
[375]:
```
from plotnine import ggplot, aes, geom_point, facet_grid, geom_abline,␣
 ↪geom_text, xlab, ylab

adjust_text_dict = {
    'expand_points': (2, 2),
    'arrowprops': {
        'arrowstyle': '-',
        'color': 'black'
    }
}

(
    ggplot(df_pred.loc[df_pred.model == 'GBR'])  # What data to use
    + geom_point(mapping=aes(x='y_actual', y='value', color='moa_final'))  #␣
 ↪What variable to use
    + facet_wrap('~variable')  # Geometric object to use for drawing
    + geom_abline(intercept = 0, slope = 1, linetype="dashed", size=1)
    + geom_text(mapping=aes(x='y_actual', y='value', label='drug'),
                nudge_x = 0.1, nudge_y = 0.1, size=4, adjust_text =␣
 ↪adjust_text_dict)
    + xlab('% Viability, Actual')
    + ylab('% Viability, Predicted')
)
```



```
[375]: <ggplot: (110059908253)>
```

```
[477]: ## create another column (idx) reordered by mean by drug
df_temp = pd.DataFrame(df_pred.groupby('drug').delta.mean())
df_temp.sort_values(by='delta', ascending=False, inplace=True)
df_temp.reset_index(drop=False, inplace=True)
df_temp.reset_index(drop=False, inplace=True)
df_temp.drop(columns=['delta'], inplace=True)
df_temp.columns = ['idx', 'drug']
df_temp.idx = df_temp.idx + 1

## merge to add idx column
df_pred = df_pred.merge(df_temp,
                        left_on = "drug",
                        right_on = "drug",
                        how = "left")

## change names of variable column
# df_pred.variable.loc[(df_pred.variable == 'y_pred_bin')] = 'BoW, Binary'
# df_pred.variable.loc[(df_pred.variable == 'y_pred_count')] = 'BoW, Count'
# df_pred.variable.loc[(df_pred.variable == 'y_pred_tfidf')] = 'TF-IDF'

## merge to add freq column
df_pred = df_pred.merge(test_data.loc[:, ['drug', 'Freq']],
                        left_on = "drug",
                        right_on = "drug",
                         how = "left")

## change variable/Freq column names to method/frequency
df_pred.rename(columns={'variable':'method', 'Freq':'frequency'}, inplace=True)

df_pred['Model, Representation'] = df_pred.model + '; ' + df_pred.method
```

```
[478]: from plotnine import ggplot, aes, geom_boxplot, geom_jitter, scale_x_discrete, \
           theme, element_text, position_jitter

       (
           ggplot(df_pred)  # What data to use
           + geom_boxplot(mapping=aes(x='drug', y='delta', color='moa_final'))
           + geom_jitter(mapping=aes(x='drug', y='delta', color='moa_final',␣
        ↪shape='Model, Representation'),
                         position=position_jitter(0.2))
           + scale_x_discrete(limits=list(df_temp.drug))
           + theme(axis_text_x=element_text(rotation=90, hjust=1))
       )
```



[478]:
```
<ggplot: (110061879456)>
```

13 NOT IN USE

13.1 Sentiment Analysis

Adopted from here

https://github.com/watson-developer-cloud/python-sdk/blob/master/examples/natural_language_understandin
https://medium.com/@MissAmaraKay/watson-services-username-password-vs-api-key-1806698316be
https://cloud.ibm.com/docs/account?topic=account-iamtoken_from_apikey

[378]:
```
## function used to analyze text sentiment from dataframe
# def analyze_text(input_text, analyzer):
#     if analyzer == 'VADER':
#         result = analyzer.polarity_scores(input_text)
#         score = results['compound']
#     else:
#         score = TextBlob(input_text).sentiment.polarity

#     if score > 0:
#         result = 1
#     else:
#         result = 0
#     return result
```

[ ]:
```
## IBM-Watson sentiment analyzer
# natural_language_understanding = NaturalLanguageUnderstandingV1(
#     version='2018-03-16')
# natural_language_understanding.set_service_url('https://gateway.
↪watsonplatform.net/natural-language-understanding/api')
```

13.1.1 VADER

[171]:
```
## VaderSentiment analyzer
analyzer = SentimentIntensityAnalyzer()
```

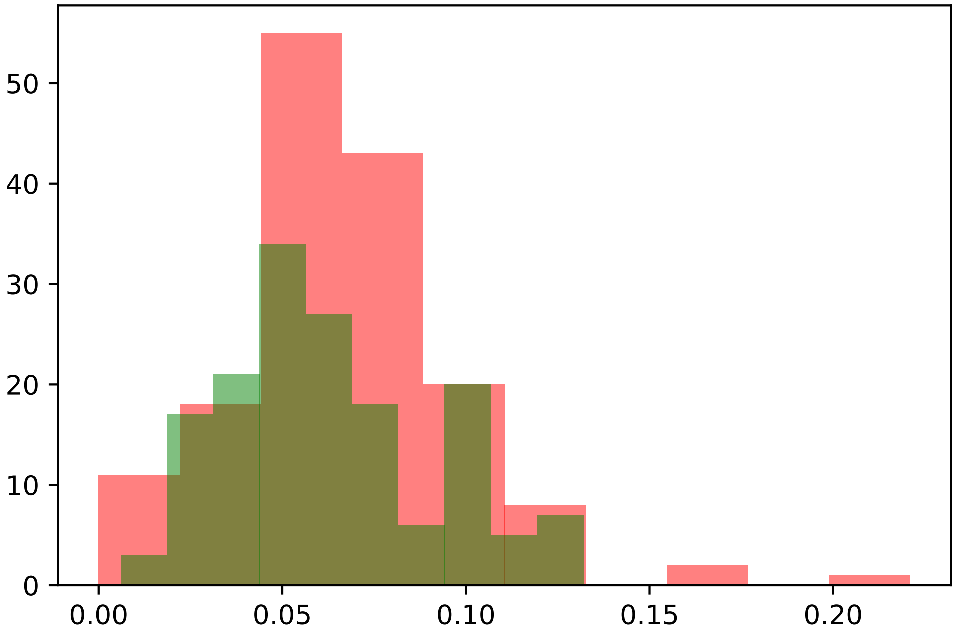
[212]:
```
vader_series = df_combo['abstract'].apply(SentimentIntensityAnalyzer().
↪polarity_scores)
# df_combo['vader'] = vader_series.apply(lambda x: x['compound'])
```

[213]:
```
vader_series[0]
```

[213]:
```
{'neg': 0.048, 'neu': 0.857, 'pos': 0.095, 'compound': 0.901}
```

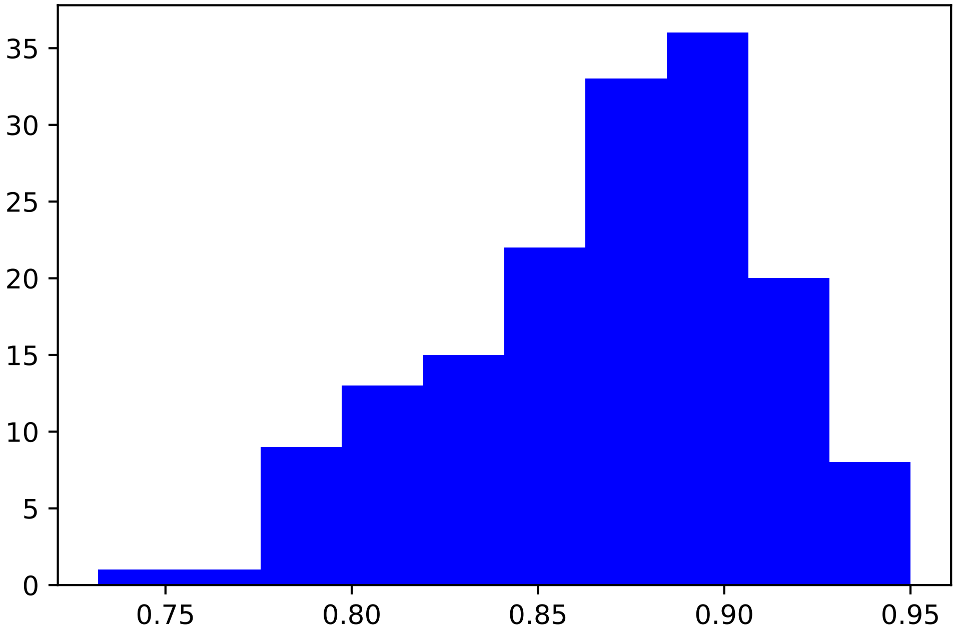
[214]:

```
plt.hist(vader_series.apply(lambda x: x['neg']), color = 'red', alpha = 0.5);
plt.hist(vader_series.apply(lambda x: x['pos']), color = 'green', alpha = 0.5);
```

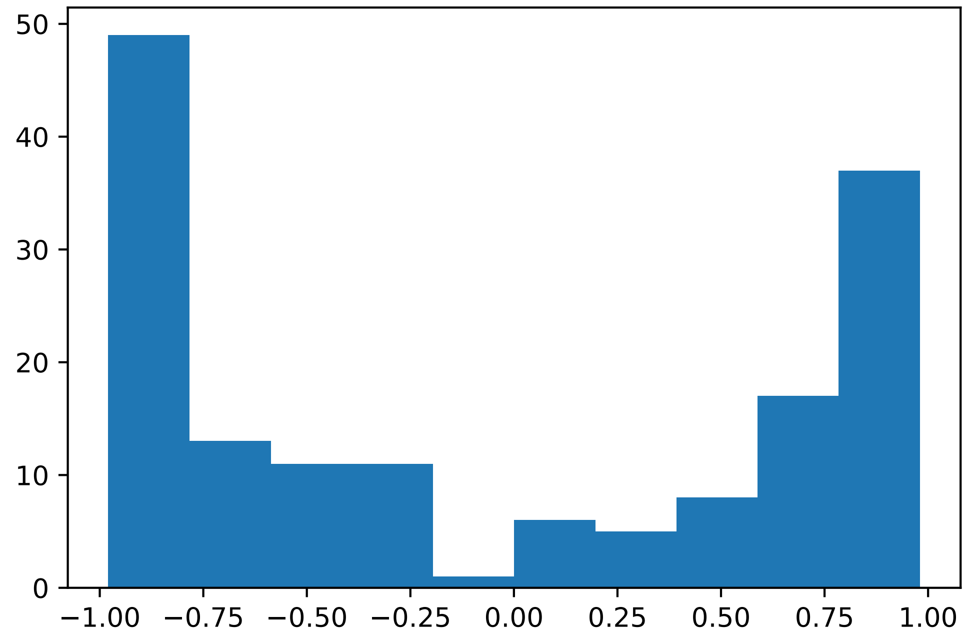


[215]:

```
plt.hist(vader_series.apply(lambda x: x['neu']), color = 'blue');
```



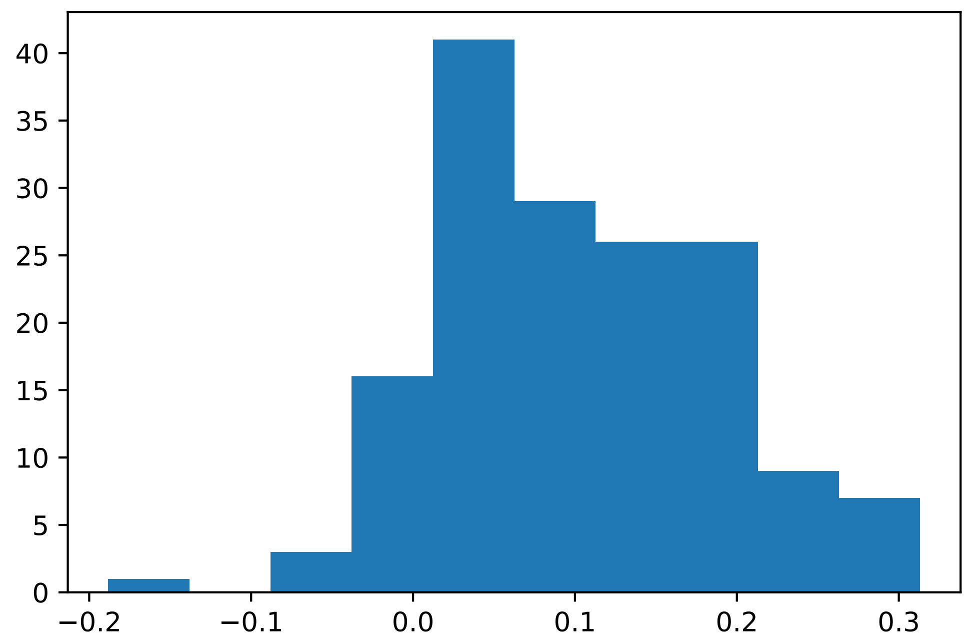
[216]:
```
plt.hist(vader_series.apply(lambda x: x['compound']));
```



13.1.2 TextBlob for Consensus

[219]:
```
textblob_series = df_combo['abstract'].apply(lambda x: TextBlob(x).sentiment.
 ↪polarity)
```

[220]:
```
plt.hist(textblob_series);
```



[432]:
```
def compare_sent(vader, textblob):
    if vader*textblob >= 0:
        temp = 1
    else:
        temp = 0
    return temp
```

13.1.3 Compare Sentiment Analysis to % Viability

[274]:
```
df_melt = df_combo.copy()

scaler = StandardScaler()

df_sent = pd.DataFrame({'vader': vader_series.apply(lambda x: x['compound']),
                       'textblob': textblob_series})

df_sent = scaler.fit_transform(df_sent)

df_melt['vader'] = df_sent[:, 0]
df_melt['textblob'] = df_sent[:, 1]
df_melt.head()
```

[274]:
```
   std_name symptom_name    median      mean       min       max disease_name  \
0  apatinib   meningioma  0.956971  0.941082  0.793878  1.063913          NF2
1  apatinib   meningioma  0.956971  0.941082  0.793878  1.063913          NF2
```

```
2  apatinib   meningioma  0.956971  0.941082  0.793878  1.063913          NF2
3  apatinib   schwannoma  0.589936  0.365289  0.001806  0.614045          NF2
4  apatinib   schwannoma  0.589936  0.365289  0.001806  0.614045          NF2

                                          abstract  abstract_no     vader  \
0  loss of the tumor suppressor merlin causes dev…          683  1.266255
1  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549 -1.078984
2  introduction: epidermal growth factor receptor…         2843  1.360106
3  loss of the tumor suppressor merlin causes dev…          683  1.266255
4  neurofibromatosis type 2 ( nf2; mim # 101000) …         1549 -1.078984

   textblob
0  1.043571
1 -0.985514
2 -1.493368
3  1.043571
4 -0.985514
```

[275]:

```
df_melt = pd.melt(df_melt[['std_name', 'symptom_name', 'median', 'mean', 'min',␣
 ↪'max', 'vader', 'textblob']],
                  id_vars = ['std_name', 'symptom_name', 'vader', 'textblob'])
df_melt.columns = ['drug', 'condition', 'vader', 'textblob', 'sum_stat',␣
 ↪'sum_value']

df_melt = pd.melt(df_melt, id_vars = ['drug', 'condition', 'sum_stat',␣
 ↪'sum_value'])

df_melt.head()
```

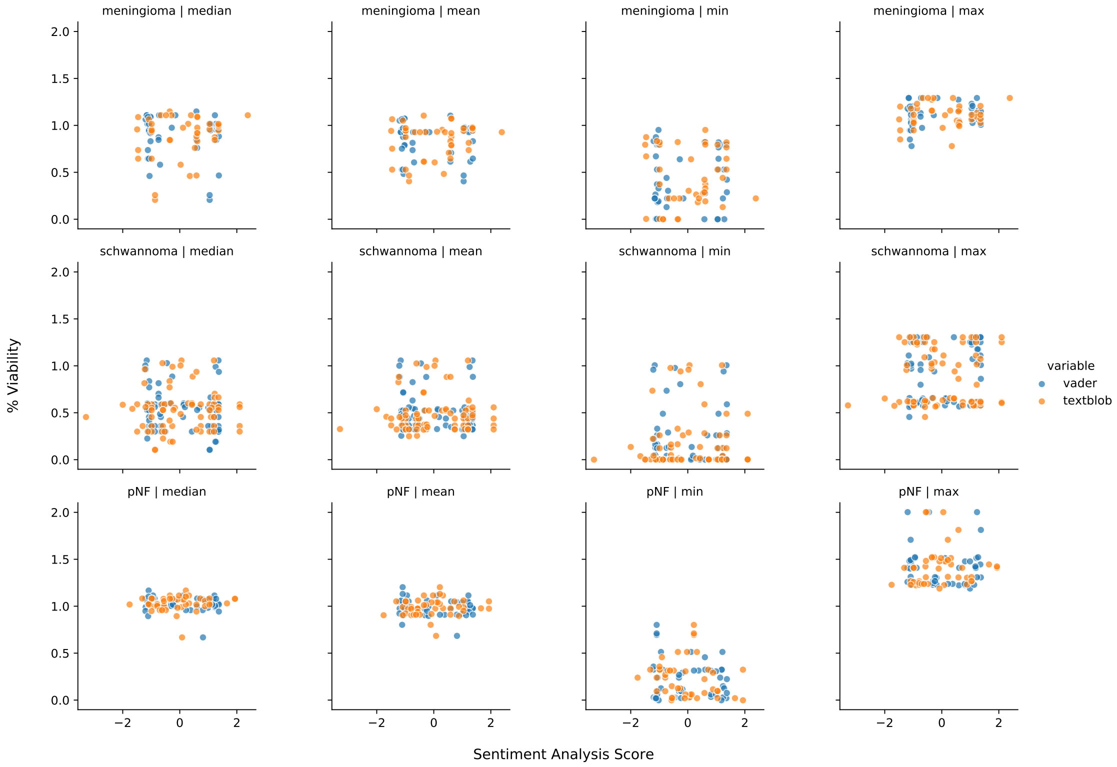
[275]:

```
       drug   condition sum_stat  sum_value variable     value
0  apatinib  meningioma   median   0.956971    vader  1.266255
1  apatinib  meningioma   median   0.956971    vader -1.078984
2  apatinib  meningioma   median   0.956971    vader  1.360106
3  apatinib  schwannoma   median   0.589936    vader  1.266255
4  apatinib  schwannoma   median   0.589936    vader -1.078984
```

[289]:

```
g = sns.FacetGrid(df_melt, row = 'condition', col = 'sum_stat', hue =␣
 ↪'variable');
g.map(sns.scatterplot, 'value', 'sum_value', alpha=.7);
g.set_titles(row_template = '{row_name}', col_template = '{col_name}');
g.set_axis_labels('Sentiment analysis score', '% viability');
g.add_legend();

#this surpresses the x- and y-labels on each axes of the bottom/leftmost column
g.set_axis_labels('', '')

# overall ylabel
```

```
g.fig.text(x=0, y=0.5,
           verticalalignment='center', #make sure it's aligned at center␣
 ↪vertically
           s='% Viability', #this is the text in the ylabel
           size=12, #customize the fontsize if you will
           rotation=90) #vertical text

#overall xlabel
g.fig.text(x=0.5, y=0,
           horizontalalignment='center', #make sure it's aligned at center␣
 ↪horizontally
           s='Sentiment Analysis Score', #this is the text in the xlabel
           size=12)

# plt.tight_layout()

plt.savefig("../images/Fig1.png", dpi=410);
```



13.1.4 Combine VADER and TextBlob

```
[437]: df_abstract_drug_2['consensus'] = [compare_sent(x, y) for x, y in␣
        ↪zip(df_abstract_drug_2['vader'], df_abstract_drug_2['textblob'])]
```

```
[439]: df_abstract_drug_2.to_csv('../assets/drug_abstracts.csv', index=False)
```

13.2 Drug Annotations

13.2.1 MedChem Annotations

```
[6]: df_moa_1 = pd.read_csv('../assets/moa/medchem.csv', header=0, encoding =␣
      ↪"ISO-8859-1")
```

```
[7]: df_moa_1 = clean_names(df_moa_1)
     df_moa_1.rename(columns = {'chemcial_name':'chemical_name'}, inplace = True)
     df_moa_1.chemical_name = df_moa_1.chemical_name.str.rsplit("(", n=1,␣
      ↪expand=True).iloc[:, 0]
     df_moa_1.head()
```

```
[7]:        plate well _catalog_number  chemical_name   _cas_number  \
     0   HY-L009-1  A02      HY-100006A      MRT68921           NaN
     1   HY-L009-1  A03        HY-10005   Flavopiridol   146426-40-6
     2   HY-L009-1  A04        HY-10006  Flavopiridol    131740-09-5
     3   HY-L009-1  A05        HY-10008        SNS-032   345627-80-7
     4   HY-L009-1  A06       HY-100114          TA-01  1784751-18-3

                                     target  \
     0                                 ULK;
     1                                 CDK;
     2                                 CDK;
     3                                 CDK;
     4  Casein Kinase; Casein Kinase; p38 MAPK;

                                             pathway  \
     0                                    Autophagy;
     1                         Cell Cycle/DNA Damage;
     2                         Cell Cycle/DNA Damage;
     3                         Cell Cycle/DNA Damage;
     4  Cell Cycle/DNA Damage; Stem Cells/Wnt; MAPK/ER…

                                   alternative_names  \
     0    MRT 68921 hydrochloride;MRT-68921 hydrochloride
     1                      L868275; HMR-1275; Alvocidib
     2  HL 275;NSC 649890;MDL 107826A;FLAVOPIRIDOL HCL…
     3     BMS-387032;SNS 032;SNS032;BMS 387032;BMS387032
     4                                       TA01;TA 01
```

```
                              biological_description       mwt       formula  \
0  MRT68921 hydrochloride is the most potent inhi…  471.0380   C25H35ClN6O
1  Flavopiridol competes with ATP to inhibit CDKs…  401.8402   C21H20ClNO5
2  Flavopiridol hydrochloride competes with ATP t…  438.3011  C21H21Cl2NO5
3  SNS-032(BMS-387032) is a potent inhibitor of c…  380.5280  C17H24N4O2S2
4  TA-01 potently inhibits CK1?, CK1?,and p38? (I…  351.3246    C20H12F3N3

                                        solubility research_area
0                                   H2O: ? 31mg/mL        Cancer
1  DMSO ?14mg/mL Water <1.2mg/mL Ethanol ?7.8mg/mL        Cancer
2   DMSO ?85mg/mL Water ?85mg/mL Ethanol ?9.3mg/mL        Cancer
3   DMSO ?73mg/mL Water <1.2mg/mL Ethanol ?73mg/mL        Cancer
4                                    10 mM in DMSO        Cancer
```

13.2.2 Thesis Annotations

[8]:
```
df_moa_2 = pd.read_csv('../assets/moa/thesis.csv', header=0)
```

[9]:
```
df_moa_2.head()
```

[9]:
```
                                    Drugs  MOA Target Phase pert_id  \
0                            (-)-cotinine  NaN    NaN   NaN     NaN
1                 (-)-gallocatechin gallate  NaN    NaN   NaN     NaN
2                                  (-)-jq1  NaN    NaN   NaN     NaN
3  (+)-3-hydroxy-n-methylmorphinan d-tartrate  NaN    NaN   NaN     NaN
4                                  (+)-jq1  NaN    NaN   NaN     NaN

  moa_brd      moa_final     moa_manual
0     NaN            NaN            NaN
1     NaN            NaN            NaN
2     NaN  BET inhibitor  BET inhibitor
3     NaN            NaN            NaN
4     NaN  BET inhibitor  BET inhibitor
```

[10]:
```
df_moa_2.Drugs[1:20]
```

[10]:
```
1                      (-)-gallocatechin gallate
2                                        (-)-jq1
3     (+)-3-hydroxy-n-methylmorphinan d-tartrate
4                                        (+)-jq1
5                                  (e)-capsaicin
6                             (s)-(-)-bay k 8644
7                              1-benzylimidazole
8                                        10-debc
9                                       11k-629s
10                                      12k-516s
11                                      12k-612s
```

```
12                                      12k-613s
13                                     1391-0741
14                                     1483-0018
15                                     1495-0136
16                     15-delta-prostaglandin-j2
17                                         1541b
18                     16-beta-bromoandrosterone
19                 17-beta-estradiol 17-valerate
Name: Drugs, dtype: object
```

13.3 Literature Summary

13.3.1 Drugs from MedChem

[165]:

```python
## replace - with ""
chem_list_1 = df_moa_1.chemical_name.replace("-", "", regex = True)
## set all values lower case
chem_list_1 = chem_list_1.str.lower()
## remove white spaces
chem_list_1 = chem_list_1.str.strip()
## remove duplicates
chem_list_1 = list(set(chem_list_1.to_list()))
```

[197]:

```python
idx_list_1 = []

for n in chem_list_1:
    temp_list = abstract_series.str.find(n).to_list()
    temp_idx = [i for i, j in enumerate(temp_list) if j >= 0]
    idx_list_1.append(temp_idx)

idx_drug_1 = [i for i, j in enumerate(idx_list_1) if j != []]
drug_list_1 = [chem_list_1[i] for i in idx_drug_1]
idx_list_1 = [i for i in idx_list_1 if i != []]
```

[176]:

```python
print(len(chem_list_1))

print(chem_list_1.index("pd0325901"))
print(chem_list_1.index("selumetinib"))

print(chem_list_1[189])
print(chem_list_1[176])
```

```
533
189
176
pd0325901
selumetinib
```

[204]:

```
del idx_list_1[drug_list_1.index("bio")]
del drug_list_1[drug_list_1.index("bio")]
```

[205]:

```
print(idx_list_1)
print()
print(drug_list_1)
```

```
[[3558], [1528, 3295], [1915], [45, 128, 192, 452, 525, 652, 659, 968, 1199,
1274, 1283, 1721, 1965, 2278, 2556, 2570, 2602, 2669, 2857, 2922, 3285, 3406,
3783, 3819, 4028, 4045, 4790, 4809, 4959, 5026, 5072, 5136, 5180, 5284], [4424],
[4045], [2038], [4045], [3146, 3278, 4387], [4977], [1528, 2270, 3295, 4045],
[4369], [2130], [4019], [71, 468, 1694, 2033, 3302, 5158], [779, 968, 1786,
2161, 2622, 3159, 3718, 4444, 5309], [4045, 4841], [557, 619, 1842, 1915, 2204,
2268, 3146, 4090, 4572, 4601, 4833, 4938, 5226, 5528], [430, 689, 964, 1794,
1915, 2589, 2963, 2997, 3146, 3159, 3257, 3302, 4077, 5220], [35, 361, 860,
2142, 2224, 3418], [49, 339, 2471, 3309, 4304, 5308, 5537], [545, 2806], [762,
1721, 1959, 2630, 2675, 2783, 2970, 3136, 3663, 4189], [2038], [1528, 3743],
[784, 1925, 2556, 2589, 3487, 4790, 4866], [3478], [2993, 4938], [608, 1485,
1721, 2675, 2905, 4082, 4106, 4189, 4529, 5055], [963, 1415, 1703, 3204],
[4045], [430, 1568, 5226], [3302], [762, 1721, 1959, 2630, 2675, 2783, 2970,
3136, 3663, 4189], [2097, 2139, 2161, 3718], [4416], [3731, 4045], [3193], [978,
2506, 2540, 2603, 2697, 2964, 3075, 3848, 4030, 5024, 5190], [3091, 3701],
[3626, 4066, 4158, 4263], [659, 968, 1689, 2753, 3663, 4045], [430, 762, 968,
1484, 1513, 1694, 1721, 3013, 4061, 4387, 4647, 5547], [416], [781, 4261, 4474,
5145], [1143], [1344, 3185, 4978], [2556, 2593, 4790], [2350], [399], [3701],
[4045]]

['sp600125', 'saracatinib', 'cobimetinib', 'imatinib', 'as605240', 'crenolanib',
'ag1478', 'linsitinib', 'vemurafenib', 'id8', 'dasatinib', 'cx4945', 'dmat',
'gdc0980', 'braf inhibitor', 'selumetinib', 'ponatinib', 'pd0325901',
'trametinib', 'zoledronic acid', 'pp1', 'pd98059', 'apatinib', 'poziotinib',
'cabozantinib', 'sunitinib', 'sl327', 'ly294002', 'erlotinib', 'crizotinib',
'masitinib', 'u0126', 'dabrafenib', 'lapatinib', 'ldn193189', 'pdk1 inhibitor',
'pazopanib', 'ng 52', 'mns', 'ruxolitinib', 'dph', 'nilotinib', 'sorafenib',
'cediranib', 'pp2', 'pi103', 'vandetanib', 'regorafenib', 'pf04691502',
'gsk2126458', 'tg101348', 'dovitinib']
```

13.3.2 Drugs from Thesis

[181]:

```
## replace - with ""
chem_list_2 = df_moa_2.Drugs.replace("-", "", regex = True)
## set all values lower case
chem_list_2 = chem_list_2.str.lower()
## remove white spaces
# chem_list_2 = chem_list_2.str.strip()
## remove duplicates
chem_list_2 = list(set(chem_list_2.to_list()))
```

[184]:

```
len(chem_list_2)

print(chem_list_2.index("pd0325901"))
print(chem_list_2.index("selumetinib"))

print(chem_list_2[335])
print(chem_list_2[2233])
```

```
335
2233
pd0325901
selumetinib
```

[187]:

```
print(chem_list_2.index("azd8055"))
print(chem_list_2[684])
```

```
684
azd8055
```

[298]:

```
idx_list_2 = []

for n in chem_list_2:
    temp_list = abstract_series.str.find(n).to_list()
    temp_idx = [i for i, j in enumerate(temp_list) if j >= 0]
    idx_list_2.append(temp_idx)

idx_drug_2 = [i for i, j in enumerate(idx_list_2) if j != []]
drug_list_2 = [chem_list_2[i] for i in idx_drug_2]
idx_list_2 = [i for i in idx_list_2 if i != []]
```

[299]:

```
[drug_list_2[i] for i, j in enumerate(idx_list_2) if len(j) > 20]
```

[299]:

```
['imatinib', 'rapamycin', 'c1', 'ite', 'fit', 'pit', 'dapt', 'ftt']
```

[300]:

```
temp = [drug_list_2[i] for i, j in enumerate(idx_list_2) if len(j) > 20]

## remove imatinib
del temp[0]
## remove rapamycin
del temp[0]

for n in temp:
    idx = drug_list_2.index(n)
    del idx_list_2[idx]
    del drug_list_2[idx]
```

[301]:

```
print(idx_list_2)
print()
print(drug_list_2)
```

```
[[3825], [1370, 2986], [39, 109, 402, 467, 583, 590, 870, 1075, 1142, 1150,
1549, 1777, 2060, 2313, 2353, 2415, 2588, 2651, 2977, 3085, 3426, 3459, 3651,
4351, 4369, 4507, 4568, 4670, 4711, 4802], [4335], [111], [6, 36, 45, 88, 213,
332, 426, 493, 648, 652, 667, 755, 877, 1248, 1406, 1448, 1519, 1525, 1560,
1737, 1822, 1989, 2053, 2126, 2268, 2434, 2539, 2590, 2707, 2714, 2793, 2810,
3035, 3084, 3181, 3198, 3236, 3238, 3257, 3328, 3701, 3946, 4031, 4282, 4454,
4490, 4512, 4595, 4619, 4776, 4802, 4810, 5009, 5019, 5154], [2840, 4714],
[2360], [2790], [2372, 3670], [4398], [1361, 2547, 3824, 4848, 4988], [493, 551,
1660, 1728, 1990, 2051, 2852, 3707, 4147, 4175, 4391, 4488, 4753, 5015], [2263],
[285, 2976], [1216, 2126], [285], [1147, 1214, 2760, 2793, 3441], [276, 819,
1702, 1858, 2721, 3052, 3304, 3709, 4245, 4327, 4366, 4396, 4591, 4598, 4929],
[2717, 4488], [2263], [4859], [4586], [3909], [1323], [4658], [493], [2803,
3350], [661], [3350], [2526, 4546], [3398], [5000], [4154], [551, 1570, 3562,
4753], [2991, 4679], [2852, 2971, 3976], [1370, 2053, 2986], [3643], [429],
[382, 618, 867, 1617, 1728, 2340, 2689, 2721, 2852, 2862, 2951, 2993, 3694,
4747], [43, 298, 2232, 2998, 3899, 4823, 5024], [4916], [101, 429, 484, 595,
1173, 1491, 1503, 1525, 1871, 2048, 2427, 3965, 4327, 4435, 4571, 4662, 4762],
[542, 1333, 1549, 2421, 2635, 3699, 3720, 3792, 4112, 4595], [382, 1404, 4753],
[398], [50, 168, 202, 337, 821, 903, 1232, 1361, 1921, 2267, 2580, 2882, 2919,
3802], [3377], [113, 345, 4080, 4204], [598, 603, 1708, 2527, 2825, 2835, 3307,
3799, 4191, 4768, 5140], [305, 345, 1040, 1336, 1384, 1543, 1791, 1930, 2227,
2302, 2558, 4591, 4607, 4802], [590, 870, 1521, 3318], [702, 3859, 4059, 4679],
[1027], [3986, 4494], [1406], [279], [410, 3340], [6, 45, 140, 648, 1448, 1549,
1660, 1737, 2421, 2707, 2845, 2993, 3318, 3573, 3792, 4776, 5009], [1848, 4743],
[202, 837, 1467, 2635, 4050, 4467], [3393], [1991], [279, 3899, 4154, 4271,
4858], [700, 870, 1609, 1952, 2372, 2862, 3364, 4031, 4824], [3562], [3792],
[4342], [704, 1737, 2313, 2340, 3155, 4351, 4422], [896], [1260], [2263],
[2993], [595, 819, 2427, 4531, 4929], [1848, 4743], [2526], [3824], [2392,
3562], [1205, 2886, 4525], [2622, 4039, 4754, 4899], [2313, 2344, 4351], [3946],
[1641, 2232, 3986, 4494], [4011], [285, 1970, 2289], [4229], [4040], [484,
4762], [1871], [870, 1609, 1728, 2372, 3364], [542], [6, 88, 116, 1248, 2263,
2590, 2861, 3198, 4030, 4802, 5017, 5019], [484, 2540], [2544], [1370, 3389],
[866, 1271, 1533, 2905], [283], [161], [1233], [36, 4724], [1232, 1361, 2512,
3454, 3824, 4832, 4988], [35], [683, 1549, 1771, 2380, 2421, 2696, 2843, 3318,
3792], [1895, 1932, 1952, 3364], [896, 4354], [1212], [4498], [3090], [382, 683,
870, 1332, 1358, 1525, 1549, 2733, 3976, 4219, 5033], [4498], [542], [819,
4929], [355], [1944], [398, 402, 1246, 1846, 3889, 4743], [877, 3397]]

['calcitriol', 'saracatinib', 'imatinib', 'coumarin', 'agk2', 'rapamycin',
'tacrolimus', 's1071', 'raclopride', 'neca', 'ponatinib', 'testosterone',
'pd0325901', 'ivermectin', 'lamotrigine', 'verteporfin', 'carbamazepine',
'simvastatin', 'vincristine', 'ly294002', 'isotretinoin', 'nsc23766',
'chloramphenicol', 'vinorelbine', 'irbesartan', 'necrostatin1', 'azd8055',
'ruxolitinib', 'ryanodine', 'tg101348', 'rolipram', 'dpn', 's1170',
'epigallocatechin', 'retinoic acid', 'nifedipine', 'vemurafenib', 'dasatinib',
'gdc0980', 'compound d', 'trametinib', 'pp1', 'tranilast', 'doxorubicin',
'erlotinib', 'u0126', 'lenalidomide', 'progesterone', 'pazopanib', 'tms', 'cdc',
'lovastatin', 'nilotinib', 'pp2', 'pi103', 'pp30', 'torin1', 'acetylcysteine',
'celecoxib', 'everolimus', 'hydrocortisone', 'rutin', 'resveratrol', 'levodopa',
'curcumin', 'selumetinib', 'cytarabine', 'nimodipine', 'ganciclovir',
'sunitinib', 'mg132', 'evista', 'tretinoin', 'dabrafenib', 'etoposide',
'cortisone', 'forskolin', 'letrozole', 'fludarabine', 'vandetanib', 'capsaicin',
'regorafenib', 'cucurbitacini', 'pp3', 'as605240', 'levetiracetam',
'pirfenidone', 'corticosterone', 'abt737', '5fluorouracil', 'mek1/2 inhibitor',
'mifepristone', 'sirolimus', 'pd98059', 's1042', 'cabozantinib', 'crizotinib',
'flumazenil', 'mdv3100', 'methotrexate', 'doxycycline', 'estradiol', 'ctb',
'lapatinib', 'ldn193189', 'nutlin3', 'lorazepam', 'rifampicin', 'tramadol',
'sorafenib', 'ofloxacin', 'losartan', 'prednisolone', 'gsk2126458',
'risperidone', 'dexamethasone', 'artesunate']
```

[302]:

```
[drug_list_2[i] for i, j in enumerate(idx_list_2) if len(j) > 20]
```

[302]:

```
['imatinib', 'rapamycin']
```

[303]:

```
len(drug_list_2)
```

[303]:

```
117
```

[304]:

```
sum([len(i) for i in idx_list_2])
```

[304]:

```
459
```

[362]:

```
## create series with abstracts
abstract_drug_series = df_journal_en.abstract[idx_list_2[0]].
 ↪append(df_journal_en.abstract[idx_list_2[1]])

for n in range(2, len(drug_list_2)):
    abstract_drug_series = abstract_drug_series.append(df_journal_en.
 ↪abstract[idx_list_2[n]])

# print(abstract_drug_series)

## extract abstract no. for dataframe and reset index
abstract_no_list = abstract_drug_series.index.to_list()
abstract_drug_series.reset_index(drop=True, inplace=True)

##
len_list = [len(i) for i in idx_list_2]
drug_list_rep_2 = np.repeat(drug_list_2, len_list, axis=0)
```

```
df_abstract_drug_2 = pd.DataFrame({'abstract': abstract_drug_series,
                                   'abstract_no': abstract_no_list,
                                   'drug': drug_list_rep_2})

df_abstract_drug_2.head()
```

```
[362]:                                            abstract  abstract_no         drug
       0  Osteomalacia in neurofibromatosis is a rare en…         3825   calcitriol
       1  Neurofibromatosis type 2 (NF2) is a nervous sy…         1370  saracatinib
       2  Papillary renal cell carcinomas (PRCC) are a h…         2986  saracatinib
       3  In the present study, the features of gastroin…           39     imatinib
       4  Object: Angiogenesis and the platelet-derived …          109     imatinib
```

```
[439]: df_abstract_drug_2.to_csv('../assets/drug_abstracts.csv', index=False)
```