Partially Supervised Feature Selection with Regularized Linear Models

Daniel Cerdán, Fernando Freire

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1 Partially Supervised Feature Selection with Regularized Linear Models

1.1 Feature selection methods overview

This item is based con the first paper.

Goals of feature selection

Scenarios related to few tens of samples but thousands dimensions: microarray data,

1. To avoid overfiting and improve model performance, prediction performance in the case of supervised classification and better cluster detection in unsupervised scenarios.

2. To provide more efficient models

3. To gain a deeper insight into the underlying processes that generated the data. The excess of dimensionality difficult the understanding.

The problem is related to find the optimal model parameters for the optimal feature subset. So, the model parameters becomes dependent of the features selected and need to be computed more or less coupled with the guessing of model parameters.

From less (zero) to more coupled computation, we have three strategies:

1. Filter techniques. Two step process, first the filtering, then the training of the model. Take into account only the properties of the data and in some cases a certain amount of prior knowledge. Therefore it's independent of the classification method. In its most simplest form ignores dependences on the data (univariate).

   Examples: Euclidean distance, i-test Information gain, Markov blanket filter

2. Wrapper methods. Once selected a candidate subset of features, the classification model is evaluated by training and testing the model. This is iterated over a ensemble of candidate subsets, and the model (with his feature subsets) selected is the model with the best accuracy.

   It's very important to construct a good searching algorithm of subsets, in order to reduce the number of sets to model with. This methods are dependent of the classifier, model feature dependencies and have the risk to be bind to a local optima. With randomizing techniques this problem is bypassed to some extent.

   Examples: Sequential forward selection (SFS) , Sequential backward elimination, Simulated annealing, Randomized hill climbing, Genetic algorithms.

3. Embedded methods. The search of the optimal subset of features is built into the classifier. Have the advantage that they include the interaction with the classification model, while at the same time being far less computationally intensive than wrapper methods.

   Examples: Decision trees Weighted naive Bayes, Feature selection using the weight vector of SVM, AROM

1.1.1 AROM methods

The acronym derives from *Approximation of Minimization zeRO-norm*

The problem is obtain a linear predictor h, minimizing the number of independent variables (features) without loss of accuracy:

$$h(\mathbf{x}) = sign(\mathbf{w} \cdot \mathbf{x} + b)$$

for n samples $x_i \in \mathbb{R}^n$ and m labels $y_i \in \{\pm 1\}$.
The accuracy constraint requires correspondence of sign
$sign(y_i) \cdot sign(h_i) > 0$ or in other form $y_i \cdot h_i = 1$
or less restrictive, enabling $\mathbf{w}$ to scale freely $y_i \cdot h_i \geq 1$
so

$$y_i(\mathbf{w} \cdot \mathbf{x} + b) \geq 1$$

The minimization is done with a norm defined over the vectorial space of $\mathbf{w}$. One approach is to minimize the zero-norm, that is, the number of components of the vector (number of non null w_i). But it's know to be a NP-Hard problem.

It's more adequate compute over a 1-norm or a 2-norm. In the second paper, the author deduce a suitable form for the function that could be minimized, taken into account the former constraint:

$$\sum_{j=1}^{n} ln(|w_j| + \epsilon)$$

The term ϵ is included to protect from zero values inside logarithm.
AROM methods are therefore feature selection embedded methods.

l1-AROM and **l2-AROM** (in this case by means of a 2-norm minimization) algorithms optimize this algorithm by iterative rescaling of inputs and doing a smooth feature selection since the weight coefficients along some dimensions progressively drop below the machine precision while other dimensions become more significant.

1.1.2 AROM semi-supervised

Third and Fourth papers explore a improvement of these previous described methods.

Goal

Classification of microarray data: few tens of samples against several thousand dimensions (genes).

Key differential strategy

Extend AROM methods by means of partial supervision on the dimensions of a feature selection procedure. The technique proposes to use of prior knowledge to guide feature selection, but flexible enough to let the final selection depart from it if necessary to optimize the classification objective.

The preferential features are previously selected from similar datasets in large microarray databases because it's known that different sub-samples of patients lead to very similar sets of biomarkers, as expected if we are aware that the biological process explaining the outcome is common among different patients.

This datasets are called source datasets and we expect that the prediction for a similar feature vector is the same than the prediction for this vector in our dataset (the target).

In third paper prior knowledge is incorporated by biological information

So, if we have some knowledge on the relative importance of each feature (either from actual prior knowledge or from a related dataset), the supervised AROM objective can be modified by adding a prior relevance vector $\beta = [\beta_1, ..., \beta_n]$ defined over the n dimensions and where $\beta_j > 0$ is the prior relevance of the j feature.

So in this case, the function to minimize in the case of 1-norm is:

$$\sum_{j=1}^{n} \frac{1}{\beta_j} ln(|w_j| + \epsilon)$$

In the case of L2-NORM, is necessary to minimize:

$$min_{\vec{w}} \|\vec{w}\|_2^2$$

To do so, the authors Helleputte & Dupont define an iterative method over k:

1. At step $k = 0$, initialize $\vec{w}_0 = \vec{w}_0 = \vec{\beta}$
2. Iterate until convergence:
   a. Calculate $min_{\vec{w}} \|\vec{w}\|_2^2$ constrained to $y_i(\vec{w}(\vec{x}_i * \vec{w}_k) + b) \geq 1$
   b. With this $\vec{w}$ set the following iteration vector: $\vec{w}_k * \vec{w} * \vec{\beta} \to \vec{w}_{k+1}$

1.2 L2-AROM and PS-L2-AROM

Describe how the provided implementation of L2-AROM works. See [2, 3, 4] for specific details. Next, implement a variable ranking approach based on the PS-L2-AROM method, as described in [4], using the provided implementation of L2-AROM.

You should introduce the possibility in the previous implementation to specify the initial value of of the scaling vector z. By default this vector should be equal to a vector with all components equal to one. By increasing or reducing these values, one should be able to favor, or make more difficult the selection of specific features. This will lead to the method PS-L2-AROM, in which some sort of prior-knowledge about the importance of each feature can be considered.

1.2.1 Implementation

The implementation provided is based in iterative algorithm showed at the end of the previous section but without introduction of previous knowledge. We change the notation, the iterative weight/coefficients vector is $\vec{z}_k$ replacing $\vec{w}_k$

1. At step $k = 0$, initialize
$$\vec{z}_0 = (1, ..., 1)$$
2. Iterate until convergence:
   a. Calculate
   $$min_{\vec{w}} \|\vec{w}\|_2^2 \ constrained\ to : y_i(\vec{w}(\vec{x}_i * \vec{z}_k) + b) \geq 1$$
   b. With this $\vec{w}$ set the following iteration vector:
   $$\vec{z}_k * \vec{w} \to \vec{z}_{k+1}$$

The step 2.a is implemented by a linear fit over a *SVM* algorithm.
We see it commenting over the code:

```
def variable_ranking(X, Y, C = 1, threshold = 1e-10):
"""
"""
# X is the samples*features matrix and Y the labels of each sample
```

```python
final_X = X.copy()
# Ititialization of z (equation (6)
z = np.ones(X.shape[1])

length = z.shape[0]

# Array that stores the elimination order, being the higher number the first attribute
# that is eliminated and 1 the last one
elimination_order = np.zeros(length, dtype = int)

original_feature_indices = np.arange(0, length, dtype = int)
# This is the definition of the linear classifier for the equation (7)
clf = SVC(kernel = "linear", C = C, random_state = 0)

iter_without_dropping = 0
n_removed_features = 0

# The iteration stops if there are 20 iterations not able to drop new features, and
# if the remaining number of features are less than 10
while iter_without_dropping < 20 and length > 10:

    # Fit the SVC and obtain the solution w = clf.coef_[0].
    # This is the resolution of equation (7)
    clf.fit(final_X * np.outer(np.ones(X.shape[ 0 ]), z), Y)
    # Compute the new z rescaling the coeficients, equation (8).
    z *= np.abs(clf.coef_[0])
    n_features_to_drop = np.sum(z < threshold)
    if n_features_to_drop == 0:
        iter_without_dropping += 1
    else:
        iter_without_dropping = 0
        # We filter z retaining the components with values over the threshold
        # Then we store in remove_order the positions of these components according
        # to these values, the index of the smallest, the first.
        remove_order = np.argsort(z[ z < threshold ])
        # We recompute elimination order, increasing only the indexes
        # of the features removed and
        # in the order provided by remove order,
        # so the first removed feature (that one with smallest z)
        # has a new index of 0 (in this case no modification),
        # the following and index of one, and so on
        # The values assigned are refered to a initial variable
        # n_removed_features = 0 that is incremented
        # in each step by the number of removed features in order to have unique indexes.
        elimination_order[ original_feature_indices[ z < threshold ][ remove_order ] ] = \
            np.arange(0, n_features_to_drop) + n_removed_features + 1
        n_removed_features += n_features_to_drop
        length -= n_features_to_drop
```

```
        # Delete from X, z and original_features the selected ones
        final_X = final_X[ :, z >= threshold ]
        original_feature_indices = original_feature_indices[ z >= threshold ]
        z = z[ z >= threshold ]

    # Removing of all remaining features (features not processed
    if length > 0:
        remove_order = np.argsort(z)
        elimination_order[ original_feature_indices[ remove_order ] ] = \
            np.arange(0, length) + n_removed_features + 1

        # The array is reversed so the more relevant features,
        # the last ones to remove, are in the first places
        # in order to ease the feature selection.
        return np.argsort(-elimination_order)
```

To introduce previous knowledge to obtain the partially supervised extension of L2-AROM algorithm it's necessary to introduce a weight vector β according to the modified equations (6) to (8)

1. At step $k = 0$, initialize

$$\vec{z}_0 = \vec{\beta}$$

2. Iterate until convergence:

   a. Calculate

$$min_{\vec{w}} \|\vec{w}\|_2^2 \; constrained \; to : y_i(\vec{w}(\vec{x}_i * \vec{z}_k) + b) \geq 1$$

   b. With this $\vec{w}$ set the following iteration vector:

$$\vec{z}_k * \vec{w} * \vec{\beta} \rightarrow \vec{z}_{k+1}$$

The modification of the previous algorithm is included in point *1.3.4 Main process* in the first method **ps_l2_arom_feature_ranking**.

1.3 Experiments of paper 4

Reproduce the experiments reported in [4]. For this, you can make use of the associated datasets which you will find in the data folder associated to this project proposal. Note that given a particular selected subset of variables, the classifier employed should be a soft-margin linear SVM with C = 1.

We are implemented all the experiments. We are going to summarize here the interesting things in the scope of the procedure and discrepancies with the results that the authors show in the paper.

Preprocessing of datasets

T-test ranking

Main process

Stability

Impact of parameter B

1.3.1 Imports and globals

Script 1.3.1 (python)

```python
import warnings
warnings.filterwarnings("ignore")
import sys
import string
import numpy as np
import pandas as pd
from sklearn.feature_selection import GenericUnivariateSelect
from sklearn.preprocessing import StandardScaler
from sklearn import metrics
from scipy import stats
from sklearn.model_selection import train_test_split
from sklearn.metrics import confusion_matrix
from sklearn.svm import SVC, LinearSVC

NROWS = sys.maxsize
PATH_DATA = './data'
VERBOSE = False
SELECT_SAMPLES = None
SELECT_FEATURES_INI = 0
SELECT_FEATURES_FIN = -1
TEST_SIZE = 0.10
B_SIZE = 10.0 # weight to assign to favored transfered features
#NUM_FEATURES_SOURCE = min(50, int((SELECT_FEATURES_FIN-SELECT_FEATURES_INI)/2))
NUM_FEATURES_SOURCE = 50
NUM_FEATURES_SELECTED = 200
NO_TRANSFER_IDX = 3
DUAL_TRANSFER_IDX = 5
RANDOM_IDX = 4
NONE_IDX = 8
NUM_FEATURES_SOURCE = 50
RANDOM_STATE = 123456
SAMPLE_NAMES = {0:'chandran', 1:'singh', 2:'welsh', 3:'no transfer', 4:'random',
                5:'singh+welsh', 6:'chandran+welsh', 7:'chandran+singh', 8:'none'}

g_B = B_SIZE # weight to assign to favored transfered features
g_k = 0 #iteration
```

1.3.2 Preprocessing datasets

Script 1.3.2 (python)

```python
def load_df(file):
    """
    Load sample files
    """
    df = pd.read_csv('./data' + '/' + file, sep=',', header=0, nrows = NROWS)
    return df
```

```
def normalize_feature_names(features):
    """
    Normalize the names of the features in order to select the common features
    """
    features_new = []
    for feature in features:
        feature_new = feature.replace('/', '@').replace('-', '@').replace('_', '@').replace('.', '@').lower()
        if feature[0] == "X":
            features_new.append(feature_new[1:])
        else:
            features_new.append(feature_new)
    return features_new

def intersect_features(df_samples):
    """
    """
    features_0 = df_samples[0].columns
    features_1 = df_samples[1].columns
    features_2 = df_samples[2].columns
    norm_features_0 = np.array(normalize_feature_names(features_0))
    norm_features_1 = np.array(normalize_feature_names(features_1))
    norm_features_2 = np.array(normalize_feature_names(features_2))
    intersect_0 = np.array([], dtype=int)
    intersect_1 = np.array([], dtype=int)
    intersect_2 = np.array([], dtype=int)
    for idx_0, feature_0 in enumerate(norm_features_0):
        idx_1 = np.where(norm_features_1 == feature_0)
        idx_2 = np.where(norm_features_2 == feature_0)
        if idx_1[0] and idx_2[0]:
            intersect_0 = np.append(intersect_0, idx_0)
            intersect_1 = np.append(intersect_1, idx_1[0])
            intersect_2 = np.append(intersect_2, idx_2[0])
        else:
            print("UnMatch", idx_0, feature_0)
    print(intersect_0.shape)
    print(intersect_0)
    print(intersect_1)
    print(intersect_2)
    df_samples_norm = []
    df_samples_norm.append(df_samples[0].iloc[:, intersect_0])
    df_samples_norm.append(df_samples[1].iloc[:, intersect_1])
    df_samples_norm.append(df_samples[2].iloc[:, intersect_2])
    return df_samples_norm


df_samples = []
for file in ['chandran.csv','singh.csv', 'welsh.csv']:
    df_samples.append(load_df(file))
    display(df_samples[-1].head())
```

```python
df_samples_norm = intersect_features(df_samples)

# Standardize the 0 label as -1 in dataset 1
mask = df_samples_norm[1]["Y"] == 0
df_samples_norm[1].loc[mask, "Y"] = -1

for i in range(3):
    display(df_samples_norm[i].head())
```

```
   X100_g_at  X1000_at  X1001_at  X1002_f_at  X1003_s_at  X1004_at  X1005_at  \
0   7.234793  6.494211  4.853264    3.527822    5.575283  5.630715  7.070994
1   6.967237  6.632175  4.320490    3.535030    5.505270  5.173343  7.826527
2   7.026961  6.510959  4.267634    3.387379    5.906008  5.321219  7.857653
3   7.123875  6.155900  4.114608    3.380995    5.891499  5.602339  8.285221
4   7.182206  6.237578  4.194653    3.380361    5.511587  5.383889  8.941296

   X1006_at  X1007_s_at  X1008_f_at  ...  AFFX.ThrX.5_at  AFFX.ThrX.M_at  \
0  3.586507    8.607721    8.376150  ...        4.124928        3.130851
1  3.470474    6.871599    8.732676  ...        4.089809        3.030838
2  3.292397    7.521978    8.636165  ...        3.693827        2.755653
3  3.636381    8.148127    8.472201  ...        4.345752        3.122182
4  3.331588    8.257033    8.700136  ...        4.016990        2.956002

   AFFX.TrpnX.3_at  AFFX.TrpnX.5_at  AFFX.TrpnX.M_at  AFFX.YEL002c.WBP1_at  \
0         2.983105         3.286748         3.632831              3.200749
1         2.710369         3.204168         3.721313              3.080551
2         2.526112         3.254250         3.362329              2.862432
3         2.656120         3.530544         3.515947              3.026449
4         2.622684         3.263552         3.606437              3.035578

   AFFX.YEL018w._at  AFFX.YEL021w.URA3_at  AFFX.YEL024w.RIP1_at  Y
0          3.157482              3.572550              3.201209  1
1          2.908750              2.980353              3.264706  1
2          3.048200              3.247433              3.061890  1
3          3.231532              3.762868              3.354885  1
4          2.938062              3.156967              3.055146  1

[5 rows x 12626 columns]
```

```
   100_g_at   1000_at   1001_at  1002_f_at  1003_s_at   1004_at   1005_at  \
0  6.927460  7.391657  3.812922   3.453385   6.070151  5.527153  5.812353
1  7.222432  7.329050  3.958028   3.407226   5.921265  5.376464  7.303408
2  6.776402  7.664007  3.783702   3.152019   5.452293  5.111794  7.207638
3  6.919134  7.469634  4.004581   3.341170   6.070925  5.296108  8.744059
4  7.113561  7.322408  4.242724   3.489324   6.141657  5.628390  6.825370
```

```
   1006_at  1007_s_at  1008_f_at  ...  AFFX-ThrX-5_at  AFFX-ThrX-M_at  \
0  3.167275   7.354981   9.419909  ...        3.770583        2.884436
1  3.108708   7.391872  10.539579  ...        3.190759        2.460119
2  3.077360   7.488371   6.833428  ...        3.325183        2.603014
3  3.117104   7.203028  10.400557  ...        3.625057        2.765521
4  3.794904   7.403024  10.240322  ...        3.698067        3.026876

   AFFX-TrpnX-3_at  AFFX-TrpnX-5_at  AFFX-TrpnX-M_at  AFFX-YEL002c/WBP1_at  \
0         2.730025         3.126168         2.870161              3.082210
1         2.696578         2.675271         2.940032              3.126269
2         2.469759         2.615746         2.510172              2.730814
3         2.681757         3.310741         3.197177              3.414182
4         2.691670         3.236030         3.003906              3.081497

   AFFX-YEL018w/_at  AFFX-YEL021w/URA3_at  AFFX-YEL024w/RIP1_at  Y
0          2.747289              3.226588              3.480196  0
1          3.013745              3.517859              3.428752  1
2          2.613696              2.823436              3.049716  0
3          3.193867              3.353537              3.567482  0
4          2.963307              3.472050              3.598103  1

[5 rows x 12626 columns]


   AFFX.MurIL2_at  AFFX.MurIL10_at  AFFX.MurIL4_at  AFFX.MurFAS_at  \
0             -12               16              37              40
1               6                8              46              46
2             -55               33              14              44
3             -26                3             -10              39
4             -27                1               1              18

   AFFX.BioB.5_at  AFFX.BioB.M_at  AFFX.BioB.3_at  AFFX.BioC.5_at  \
0             269             209             197             695
1             261             215             153             676
2             570             535             378            1362
3             273             249             177             632
4             261             251             193             654

   AFFX.BioC.3_at  AFFX.BioDn.5_at  ...  X101_at  X102_at  X103_at  X104_at  \
0             748              816  ...       56       21      228       63
1             658              804  ...       36       27       93       79
2            1400             1640  ...       39       20       56       86
3             672              844  ...      100       19       78       61
4             711              788  ...       74       34       26       38

   X105_at  X106_at  X107_at  X108_g_at  X109_at  Y
0       64      -23      -94        -99      248  1
1       52       14      -70       -179      129  1
```

```
2       90      -15     -102        -89      117  1
3        9       16     -117        -64      153  1
4        7       23      -53        -66      141  1

[5 rows x 12627 columns]
```

Output

```
UnMatch 0 100@g@at
UnMatch 651 160020@at
UnMatch 652 160021@r@at
UnMatch 653 160022@at
UnMatch 654 160023@at
UnMatch 655 160024@at
UnMatch 656 160025@at
UnMatch 657 160026@at
UnMatch 658 160027@s@at
UnMatch 659 160028@s@at
UnMatch 660 160029@at
UnMatch 661 160030@at
UnMatch 662 160031@at
UnMatch 663 160032@at
UnMatch 664 160033@s@at
UnMatch 665 160034@s@at
UnMatch 666 160035@at
UnMatch 667 160036@at
UnMatch 668 160037@at
UnMatch 669 160038@s@at
UnMatch 670 160039@at
UnMatch 671 160040@at
UnMatch 672 160041@at
UnMatch 673 160042@s@at
UnMatch 674 160043@at
UnMatch 675 160044@g@at
UnMatch 12610 affx@muril2@at
(12599,)
[    1     2     3 ... 12623 12624 12625]
[    1     2     3 ... 12623 12624 12625]
[11737 11738 11739 ...    66    65 12626]
```

```
   X1000_at  X1001_at  X1002_f_at  X1003_s_at  X1004_at  X1005_at  X1006_at  \
0  6.494211  4.853264    3.527822    5.575283  5.630715  7.070994  3.586507
1  6.632175  4.320490    3.535030    5.505270  5.173343  7.826527  3.470474
2  6.510959  4.267634    3.387379    5.906008  5.321219  7.857653  3.292397
3  6.155900  4.114608    3.380995    5.891499  5.602339  8.285221  3.636381
4  6.237578  4.194653    3.380361    5.511587  5.383889  8.941296  3.331588

   X1007_s_at  X1008_f_at  X1009_at  ...  AFFX.ThrX.5_at  AFFX.ThrX.M_at  \
0    8.607721    8.376150  8.000115  ...        4.124928        3.130851
1    6.871599    8.732676  7.820364  ...        4.089809        3.030838
```

```
2    7.521978    8.636165  7.880739  ...        3.693827        2.755653
3    8.148127    8.472201  7.894054  ...        4.345752        3.122182
4    8.257033    8.700136  8.103976  ...        4.016990        2.956002

   AFFX.TrpnX.3_at  AFFX.TrpnX.5_at  AFFX.TrpnX.M_at  AFFX.YEL002c.WBP1_at  \
0         2.983105         3.286748         3.632831              3.200749
1         2.710369         3.204168         3.721313              3.080551
2         2.526112         3.254250         3.362329              2.862432
3         2.656120         3.530544         3.515947              3.026449
4         2.622684         3.263552         3.606437              3.035578

   AFFX.YEL018w._at  AFFX.YEL021w.URA3_at  AFFX.YEL024w.RIP1_at  Y
0          3.157482              3.572550              3.201209  1
1          2.908750              2.980353              3.264706  1
2          3.048200              3.247433              3.061890  1
3          3.231532              3.762868              3.354885  1
4          2.938062              3.156967              3.055146  1

[5 rows x 12599 columns]


    1000_at   1001_at  1002_f_at  1003_s_at   1004_at   1005_at   1006_at  \
0  7.391657  3.812922   3.453385   6.070151  5.527153  5.812353  3.167275
1  7.329050  3.958028   3.407226   5.921265  5.376464  7.303408  3.108708
2  7.664007  3.783702   3.152019   5.452293  5.111794  7.207638  3.077360
3  7.469634  4.004581   3.341170   6.070925  5.296108  8.744059  3.117104
4  7.322408  4.242724   3.489324   6.141657  5.628390  6.825370  3.794904

   1007_s_at  1008_f_at   1009_at  ...  AFFX-ThrX-5_at  AFFX-ThrX-M_at  \
0   7.354981   9.419909  7.697655  ...        3.770583        2.884436
1   7.391872  10.539579  8.544981  ...        3.190759        2.460119
2   7.488371   6.833428  8.448252  ...        3.325183        2.603014
3   7.203028  10.400557  7.185107  ...        3.625057        2.765521
4   7.403024  10.240322  7.163157  ...        3.698067        3.026876

   AFFX-TrpnX-3_at  AFFX-TrpnX-5_at  AFFX-TrpnX-M_at  AFFX-YEL002c/WBP1_at  \
0         2.730025         3.126168         2.870161              3.082210
1         2.696578         2.675271         2.940032              3.126269
2         2.469759         2.615746         2.510172              2.730814
3         2.681757         3.310741         3.197177              3.414182
4         2.691670         3.236030         3.003906              3.081497

   AFFX-YEL018w/_at  AFFX-YEL021w/URA3_at  AFFX-YEL024w/RIP1_at  Y
0          2.747289              3.226588              3.480196 -1
1          3.013745              3.517859              3.428752  1
2          2.613696              2.823436              3.049716 -1
3          3.193867              3.353537              3.567482 -1
4          2.963307              3.472050              3.598103  1
```

```
[5 rows x 12599 columns]
```

```
   X1000_at  X1001_at  X1002_f_at  X1003_s_at  X1004_at  X1005_at  X1006_at  \
0       269        46          68         -11       -67      2059        43
1       245        45          18         -15        44      1885        25
2       310        24          93         -30        -8       652       -52
3       328        13          41          16        38      2536       -35
4       359        40          13          -1        42      3845       -18

   X1007_s_at  X1008_f_at  X1009_at  ...  AFFX.ThrX.5_at  AFFX.ThrX.M_at  \
0        1425        1073      2317  ...             873             613
1        1313        1521      2029  ...             908             700
2        1648        1561      1287  ...            1450            1102
3        1006        1307      2921  ...             853             604
4        1009        1156      1924  ...             931             664

   AFFX.TrpnX.3_at  AFFX.TrpnX.5_at  AFFX.TrpnX.M_at  AFFX.YEL002c.WBP1_at  \
0               -2               41              -26                     5
1               -8               13              -26                    14
2                9               27               -7                    34
3               -4                8              -35                    -4
4               -3               21              -16                     5

   AFFX.YEL018w._at  AFFX.YEL021w.URA3_at  AFFX.YEL024w.RIP1_at  Y
0               -15                    75                    16  1
1                -9                   137                     5  1
2                -4                    67                    16  1
3               -15                    70                    18  1
4                 1                    43                    12  1

[5 rows x 12599 columns]
```

1.3.3 Calculate prior rankings

Script 1.3.3 (python)

```python
def split_data(df, test_size=TEST_SIZE, select_samples=SELECT_SAMPLES):
    """
    Split data
    """
    global g_k

    #print("K", g_k)

    if select_samples == None:
```

```
        labels = df.iloc[:, -1]
        features = df.iloc[:, :-1]
    else:
        labels = np.concatenate([df.iloc[:select_samples, -1],
                                 df.iloc[-select_samples:, -1]], axis = 0)

        features = np.concatenate([df.iloc[:select_samples, SELECT_FEATURES_INI:SELECT_FEATURES_FIN],
                               df.iloc[-select_samples:, SELECT_FEATURES_INI:SELECT_FEATURES_FIN]], axis = 0)

    X_train, X_test, y_train, y_test = train_test_split(features, labels, test_size=test_size,\
                                                          random_state=RANDOM_STATE + g_k)
    #print("@@@@@@", test_size,  X_train.shape)
    return X_train, X_test, y_train, y_test

def ttest(X, y):
    """
    Score statistic function for transformer GenericUnivariate
    """
    t, p = stats.ttest_ind(X[y==1] , X[y==-1], equal_var=False)
    #print('t',abs(t), 'p', p)
    return abs(t)

def ranking_ttest(X, y):
    """
    Select the features with the t
    """
    ttest_scores = ttest(X, y)
    feature_indexes = np.argsort(ttest_scores)[::-1]
    return feature_indexes

def select_combined_features(idx_source1, idx_source2, feature_rankings, num_features=NUM_FEATURES_SOURCE):
    #275 1 y 2
    #385 0 y 2
    #557 0 y 1
    for p in range(200,600):
        feature_indexes = np.intersect1d(feature_rankings[idx_source1][:p], feature_rankings[idx_source2][:p])
        if len(feature_indexes) >= num_features:
            print("p", p, len(feature_indexes))
            break
    return feature_indexes

def calculate_prior_rankings(df_samples_norm):
    """
    Calculate prior rankings
    """
    feature_rankings = []
    for idx_source in range(3):
```

```python
        X1, _, y1, _ = split_data(df_samples_norm[idx_source], test_size=0)
        scaler = StandardScaler(with_mean=False, with_std=False)
        X1_scaled = scaler.fit_transform(X1)
        feature_rankings.append(ranking_ttest(X1_scaled, y1))

    feature_rankings_2sources = []
    feature_rankings_2sources.append(select_combined_features(1, 2, feature_rankings))
    feature_rankings_2sources.append(select_combined_features(0, 2, feature_rankings))
    feature_rankings_2sources.append(select_combined_features(0, 1, feature_rankings))

    return feature_rankings, feature_rankings_2sources

feature_rankings, feature_rankings_2sources = calculate_prior_rankings(df_samples_norm)
```

Output

```
p 262 50
p 362 50
p 513 50
```

1.3.4 Main process

Script 1.3.4 (python)

```python
def ps_l2_arom_feature_ranking(X, Y, C=1, b=None, threshold=1e-10):
    """
    # X is numpy array witht the data (rows are data instances)
    # Y is a numpy vector with the class labels (-1 or 1)
    # C is the regularization coefficient of the SVM
    # b is the relevance vector
    # threshold is the threshold value to drop features in L2AROM

    # At step k = 0, initialize z = b (relevance vector)
    # Relevance vector b:
    #   Prior relevance of feature j encoded in b_j .
    #   The more (a priori) relevant feature j, the higher b_j. If no information on j, b_j
    = 1.
    """
    global g_K
    # Preserve X input
    final_X = X.copy()
    # Initialice w_k = (1,....,1)
    # At step k = 0, initialize z = (1, ..., 1) /b
    z = b.copy()
    w_new = b.copy()
    # Number of attributes
    length = z.shape[0]

    # Array that stores the elimination order, being the higher number the first attribute
    # that is eliminated and 0 the last one
```

```
    elimination_order = np.zeros(length, dtype = int)
    original_feature_indices = np.arange(0, length, dtype = int)
    clf = SVC(kernel = "linear", C = C, random_state = g_k + RANDOM_STATE)
    iter_without_dropping = 0
    n_removed_features = 0

    # Iterate until convergence
    while iter_without_dropping < 20 and length > 10:
        clf.fit(final_X * np.outer(np.ones(X.shape[ 0 ]), w_new), Y)
        # w = coef_ is the solution so z_new <- z*w*b
        #z *= np.abs(clf.coef_[0])*b # In absolute value
        #print(clf.coef_)
        w_new *= clf.coef_[0]*b
        z = abs(w_new)
        n_features_to_drop = np.sum(z < threshold)
        if n_features_to_drop == 0:
            iter_without_dropping += 1
        else:
            iter_without_dropping = 0
            remove_order = np.argsort(z[ z < threshold ])
            elimination_order[ original_feature_indices[ z < threshold ][ remove_order ] ] = \
                np.arange(0, n_features_to_drop) + n_removed_features + 1
            n_removed_features += n_features_to_drop
            length -= n_features_to_drop
            # Delete from X, z and original_features the selected attributes
            final_X = final_X[ :, z >= threshold ]
            original_feature_indices = original_feature_indices[ z >= threshold ]
            b = b[ z >= threshold ]
            w_new = w_new[ z >= threshold ]
            z = z[ z >= threshold ]

    # We remove all remaining features
    if length > 0:
        remove_order = np.argsort(z)
        elimination_order[ original_feature_indices[ remove_order ] ] = \
            np.arange(0, length) + n_removed_features + 1
    #ranking of features for more to less significance
    return np.argsort(-elimination_order)  # So array starts at 0 (python indexing)

def linearsvc_bcr(X_train_scaled_target, y_train_target, X_test_scaled_target, y_test_target,\
                  num_features_selected=NUM_FEATURES_SELECTED, transfer_indexes=[]):
    """
    """
    global g_B

    #print("Shape", X_train_scaled_target.shape)
    b = np.ones(X_train_scaled_target.shape[1])
    b[transfer_indexes] = g_B
    #print("Beta vector", b, X_train_scaled_target.shape[0])
    #print("Selected features on target", num_features_selected)
    feature_ranking = ps_l2_arom_feature_ranking(X_train_scaled_target, y_train_target, C=1,
    ↪  b=b)
```

```python

    if VERBOSE: print("Ranking by PS-L2-AROM", feature_ranking)
    ranking_selected = feature_ranking[:num_features_selected]

    # Perform
    X_train_feature_reduction = X_train_scaled_target[:, ranking_selected]
    X_test_feature_reduction = X_test_scaled_target[:, ranking_selected]
    #print(X_train_feature_reduction)
    #print(y_train)
    lin_clf = LinearSVC(C=1.0, random_state=RANDOM_STATE)
    lin_clf.fit(X_train_feature_reduction, y_train_target)

    predicted = lin_clf.predict(X_test_feature_reduction)
    if VERBOSE: print("Predicted", predicted)
    #accuracy = metrics.accuracy_score(y_test_target, predicted)
    bcr = metrics.balanced_accuracy_score(y_test_target, predicted)
    if VERBOSE: print("Accuracy", accuracy)
    return bcr, ranking_selected

def linearsvc_bcr_none(X_train_scaled_target, y_train_target, X_test_scaled_target, y_test_target,\
              num_features_selected=NUM_FEATURES_SELECTED, transfer_indexes=[]):
    """
    """
    ranking_selected = transfer_indexes[:num_features_selected]
    #print("@Selected features on target(none)", len(transfer_indexes), len(ranking_selected))

    # Perform
    X_train_feature_reduction = X_train_scaled_target[:, ranking_selected]
    X_test_feature_reduction = X_test_scaled_target[:, ranking_selected]
    #print(X_train_feature_reduction)
    #print(y_train)
    lin_clf = LinearSVC(C=1.0, random_state=RANDOM_STATE)
    lin_clf.fit(X_train_feature_reduction, y_train_target)

    predicted = lin_clf.predict(X_test_feature_reduction)
    if VERBOSE: print("Predicted", predicted)
    #accuracy = metrics.accuracy_score(y_test_target, predicted)
    bcr = metrics.balanced_accuracy_score(y_test_target, predicted)
    if VERBOSE: print("Accuracy", accuracy)
    return bcr, ranking_selected

def compute_transfer(X_train_scaled_target, X_test_scaled_target, y_train_target, y_test_target,\
                 idx_source, num_features_selected):
    """
    """
    if idx_source == NO_TRANSFER_IDX: #no transfer
        indexes = []
    elif idx_source == RANDOM_IDX:
        indexes = np.arange(X_train_scaled_target.shape[1])
```

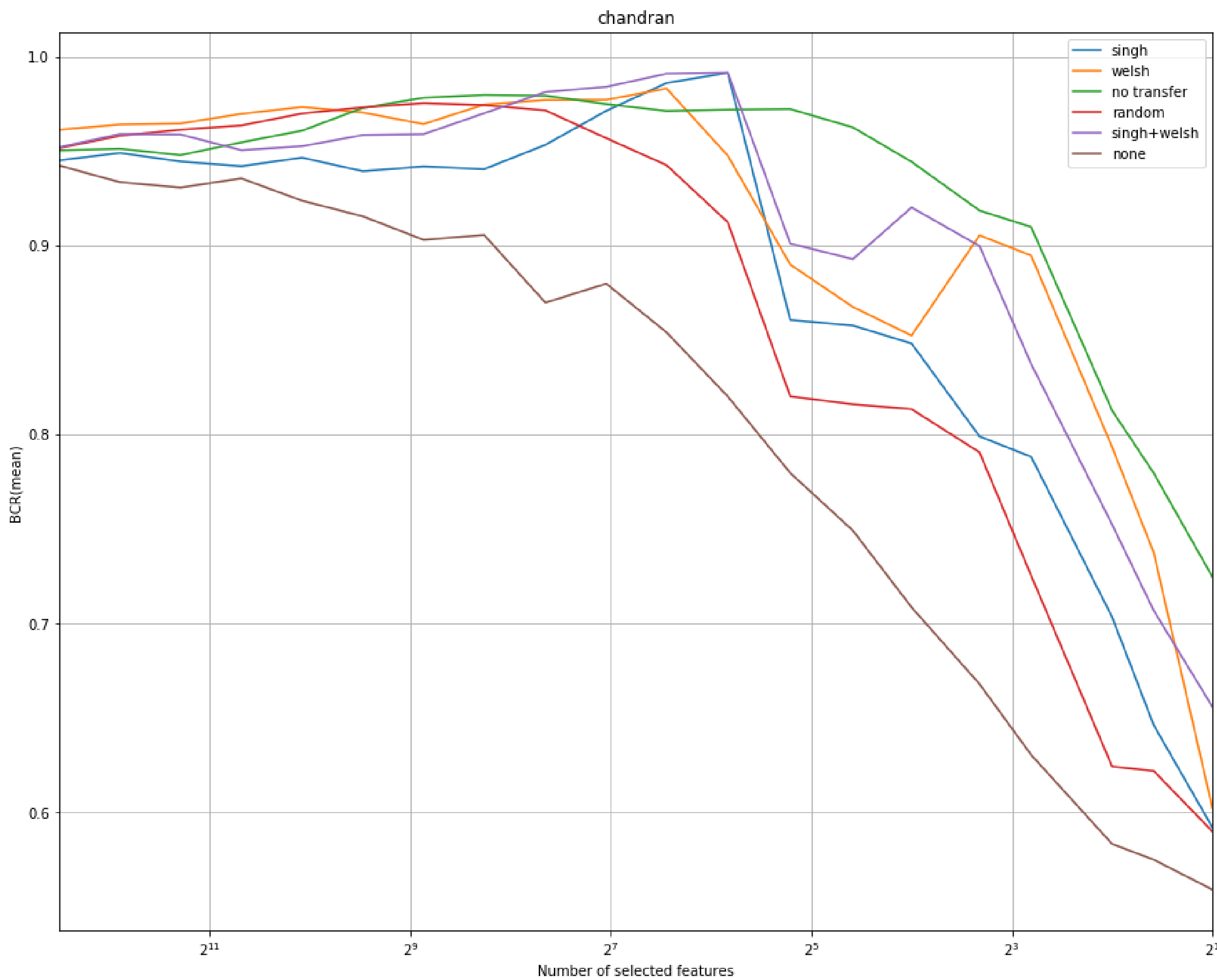
```
            np.random.shuffle(indexes)
            indexes = indexes[:NUM_FEATURES_SOURCE]
        elif idx_source == NONE_IDX:
            indexes = np.arange(X_train_scaled_target.shape[1])
            np.random.shuffle(indexes)
            indexes = indexes
        elif idx_source >= DUAL_TRANSFER_IDX:
            indexes = feature_rankings_2sources[idx_source -
             ↪  DUAL_TRANSFER_IDX][:NUM_FEATURES_SOURCE]
        else:
            indexes = feature_rankings[idx_source][:NUM_FEATURES_SOURCE]
            if VERBOSE: print("Indexes from source", y_train_target.shape[0], len(indexes))

        if idx_source == NONE_IDX:
            bcr, ranking_selected = linearsvc_bcr_none(X_train_scaled_target, y_train_target,
             ↪  X_test_scaled_target, y_test_target,\
                                num_features_selected, transfer_indexes=indexes)
        else:
            bcr, ranking_selected = linearsvc_bcr(X_train_scaled_target, y_train_target,
             ↪  X_test_scaled_target, y_test_target,\
                                num_features_selected, transfer_indexes=indexes)

        return bcr, ranking_selected

def get_target_data_sets(df_samples_norm, idx_target):
    """
    """
    X_train_target, X_test_target, y_train_target, y_test_target =
     ↪  split_data(df_samples_norm[idx_target])
    #features =
     ↪  df_samples_norm[idx_target].columns[SELECT_FEATURES_INI:SELECT_FEATURES_FIN].values
    scaler_target = StandardScaler(with_mean=False, with_std=False)
    scaler_target.fit(X_train_target)
    X_train_scaled_target = scaler_target.transform(X_train_target)
    X_test_scaled_target = scaler_target.transform(X_test_target)
    return X_train_scaled_target, X_test_scaled_target, y_train_target, y_test_target

print("Num features to feed from sources", NUM_FEATURES_SOURCE )

feature_rankings, feature_rankings_2sources = calculate_prior_rankings(df_samples_norm)

FILTER_SOURCES = [0,1,2,3,4,8]
FILTER_TARGETS = [0,1,2]
features_to_select = np.unique(np.logspace(1, 12.5, num=20, endpoint=True, base=2.0,
 ↪  dtype=int))
#features_to_select = [2,4,16,64,256,1024,4096]
bcr_list = []
for g_k in range(0, 200):
    for idx_target in FILTER_TARGETS:
        #print("TARGET", SAMPLE_NAMES[idx_target])
        X_train_scaled_target, X_test_scaled_target, y_train_target, y_test_target =\
        get_target_data_sets(df_samples_norm, idx_target)
```

```
        for idx_source in [0,1,2,3,4, DUAL_TRANSFER_IDX + idx_target, 8]:
            #if idx_source in FILTER_SOURCES and idx_source!= idx_target:
            if idx_source!= idx_target:
                print("k", g_k, "TARGET", SAMPLE_NAMES[idx_target], "SOURCE",
                 ↪  SAMPLE_NAMES[idx_source])
                for features_selected in features_to_select:
                    #print("Features",features_selected)
                    bcr, ranking_selected = compute_transfer(X_train_scaled_target,
                     ↪  X_test_scaled_target, y_train_target, y_test_target,\
                                            idx_source=idx_source,
                                             ↪  num_features_selected=features_selected)
                    bcr_list.append([SAMPLE_NAMES[idx_target], SAMPLE_NAMES[idx_source],\
                                    features_selected, bcr, ranking_selected])
                    if VERBOSE: print("Target", idx_target, "Source", idx_source,
                     ↪  "#Features",\
                                     features_selected, "BCR", bcr)

df_bcr = pd.DataFrame(bcr_list, columns=['target', 'source', 'num features', 'BCR', 'S'])
df_bcr.head()
```

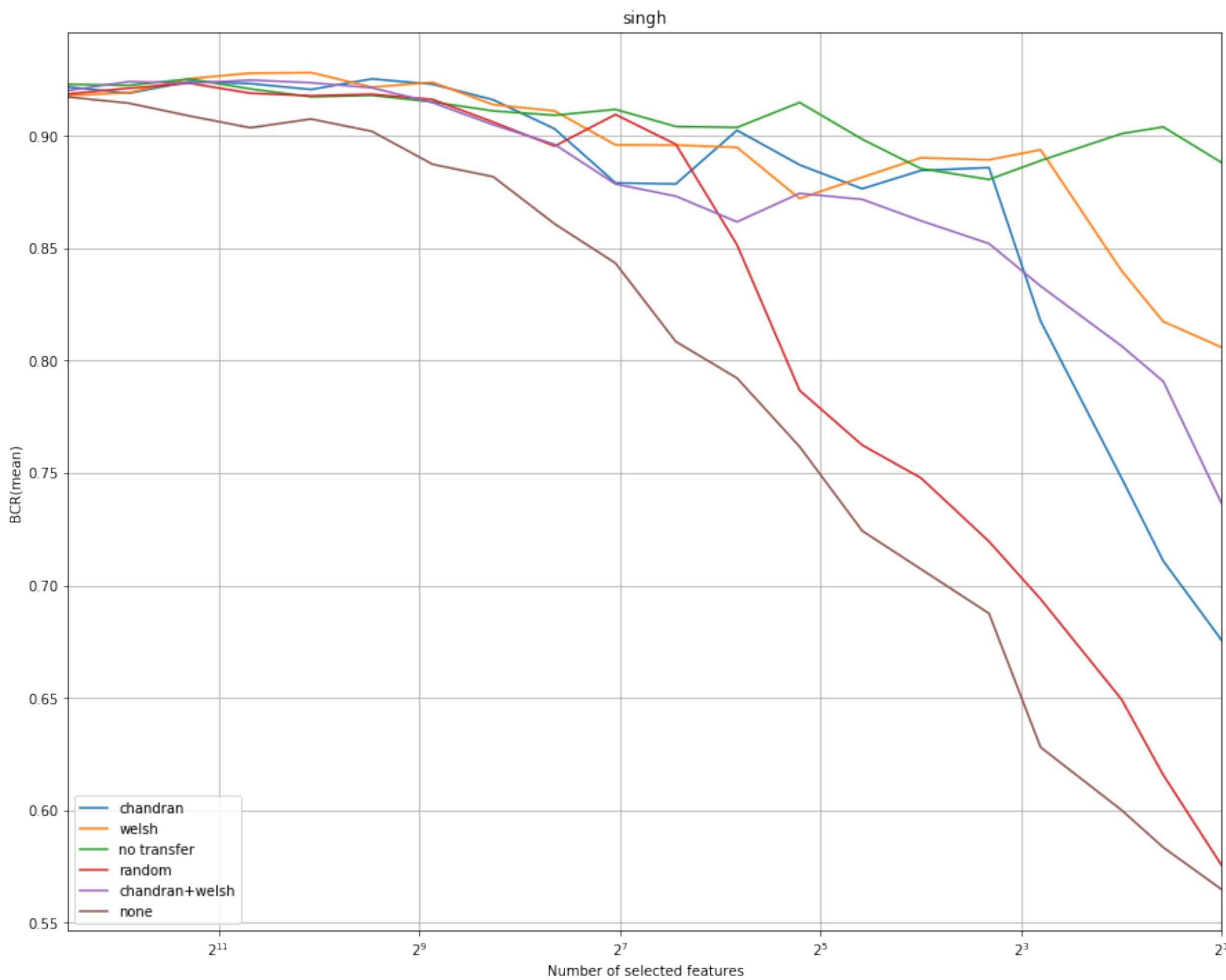
1.3.5 Plot BCR

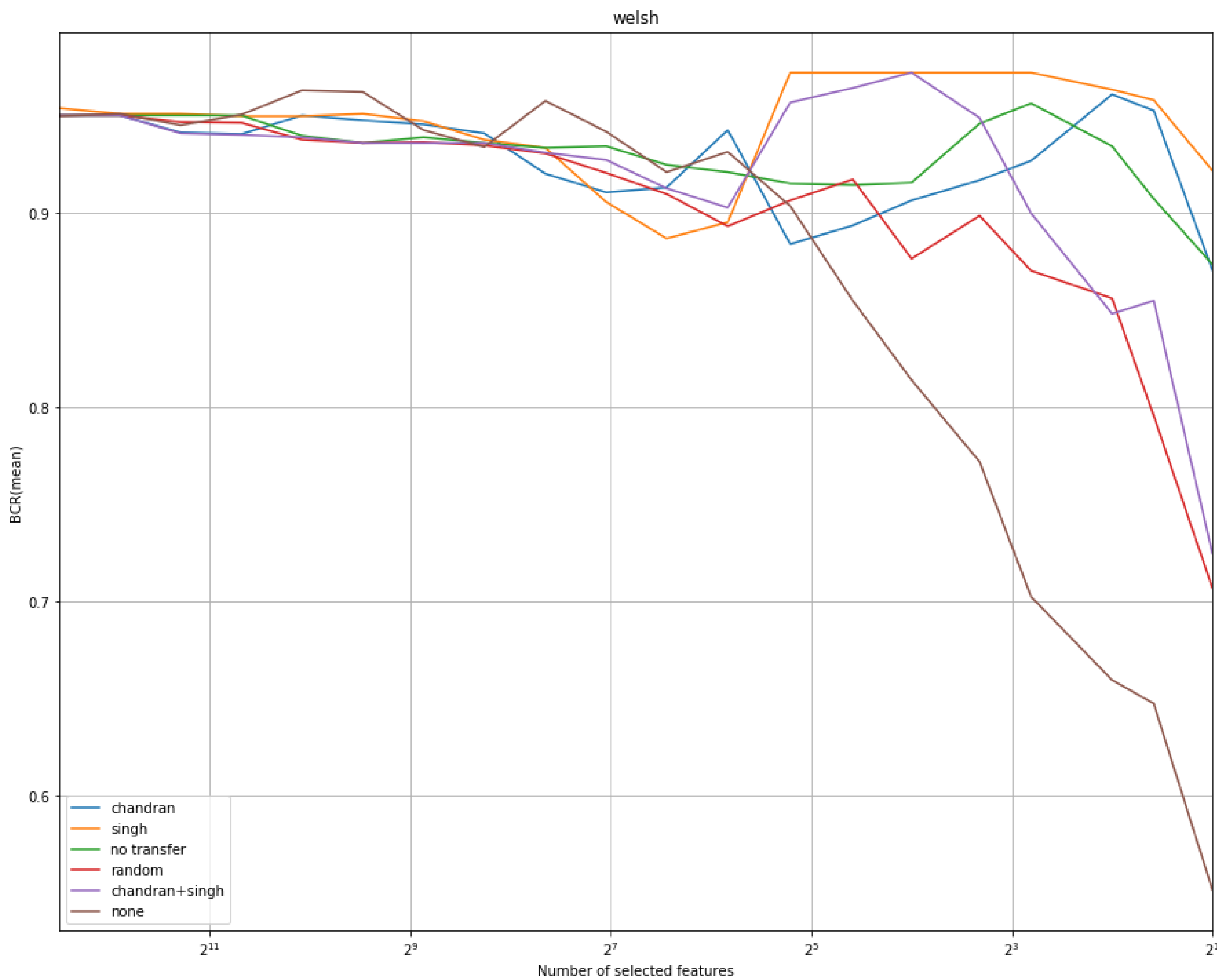
Script 1.3.5 (python)

```
import matplotlib.pyplot as plt
%matplotlib inline

idx_target = 0
df_bcr_mean = pd.DataFrame(df_bcr.groupby(['target', 'source', 'num
↪  features'])['BCR'].mean()).reset_index()
for idx_target in [0,1,2]:
    target = SAMPLE_NAMES[idx_target]
    df_target = df_bcr_mean.loc[df_bcr_mean['target'] == target]
    plt.figure(figsize=(15,12))
    plt.xscale('log', basex=2)
    for idx_source in [0,1,2,3,4, DUAL_TRANSFER_IDX + idx_target, 8]:
        #if idx_source in FILTER_SOURCES and idx_source!= idx_target:
        if idx_source!= idx_target:
            label = SAMPLE_NAMES[idx_source]
            df_source = df_target[df_target['source'] == label]
            plt.xlim(max(df_source['num features']), min(df_source['num features']))
            plt.plot(df_source['num features'], df_source['BCR'], label=label)

    plt.title(target)
    plt.xlabel("Number of selected features")
    #plt.xlim(100,400)
    #plt.xticks(df_source['num features'])
    plt.ylabel("BCR(mean)")
    plt.legend(loc = "best")
    plt.grid()
    plt.show()
```



chandran
singh
welsh
no transfer
random
singh+welsh
none
BCR(mean)
1.0
0.9
0.8
0.7
0.6
2^{11}
2^{9}
2^{7}
2^{5}
2^{3}
2^{1}
Number of selected features


singh
BCR(mean)
Number of selected features
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
2^{11}
2^{9}
2^{7}
2^{5}
2^{3}
2^{1}
chandran
welsh
no transfer
random
chandran+welsh
none



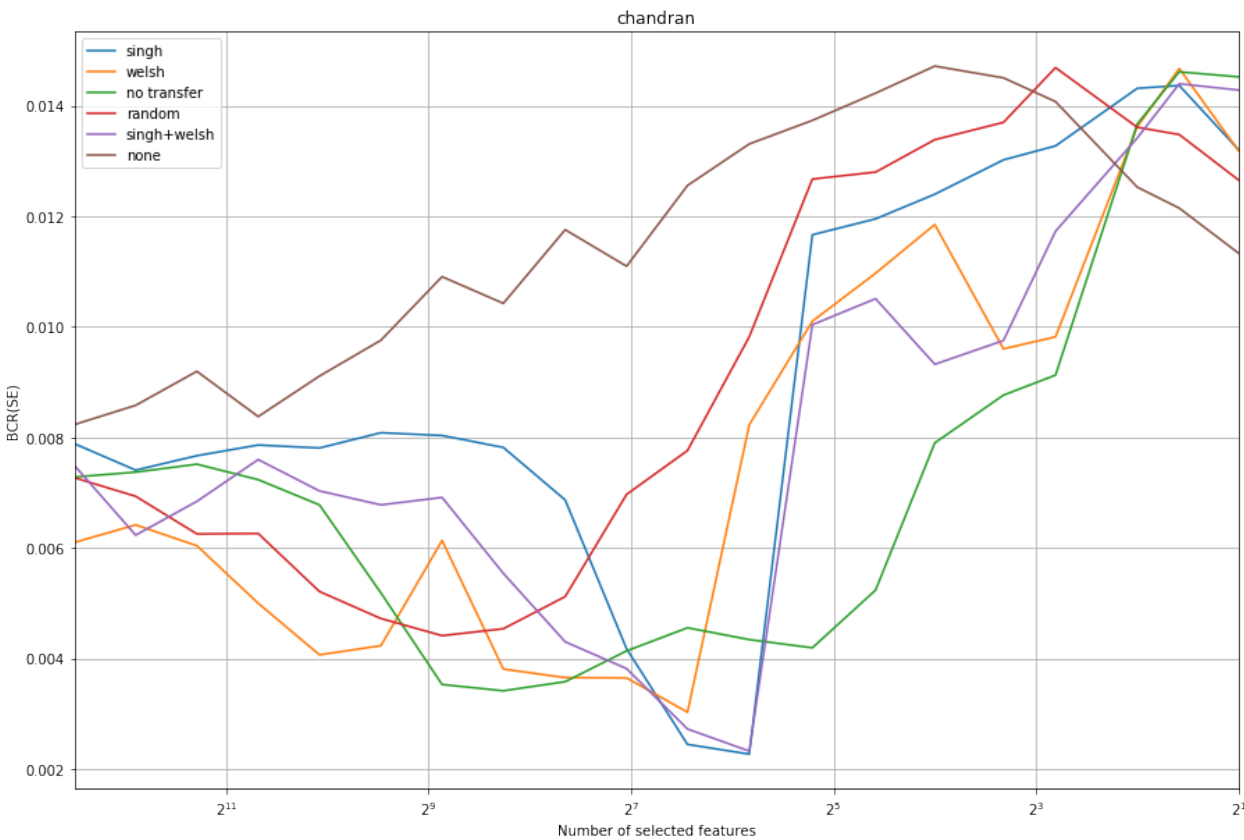
1.3.6 Plot BCR (standard error)

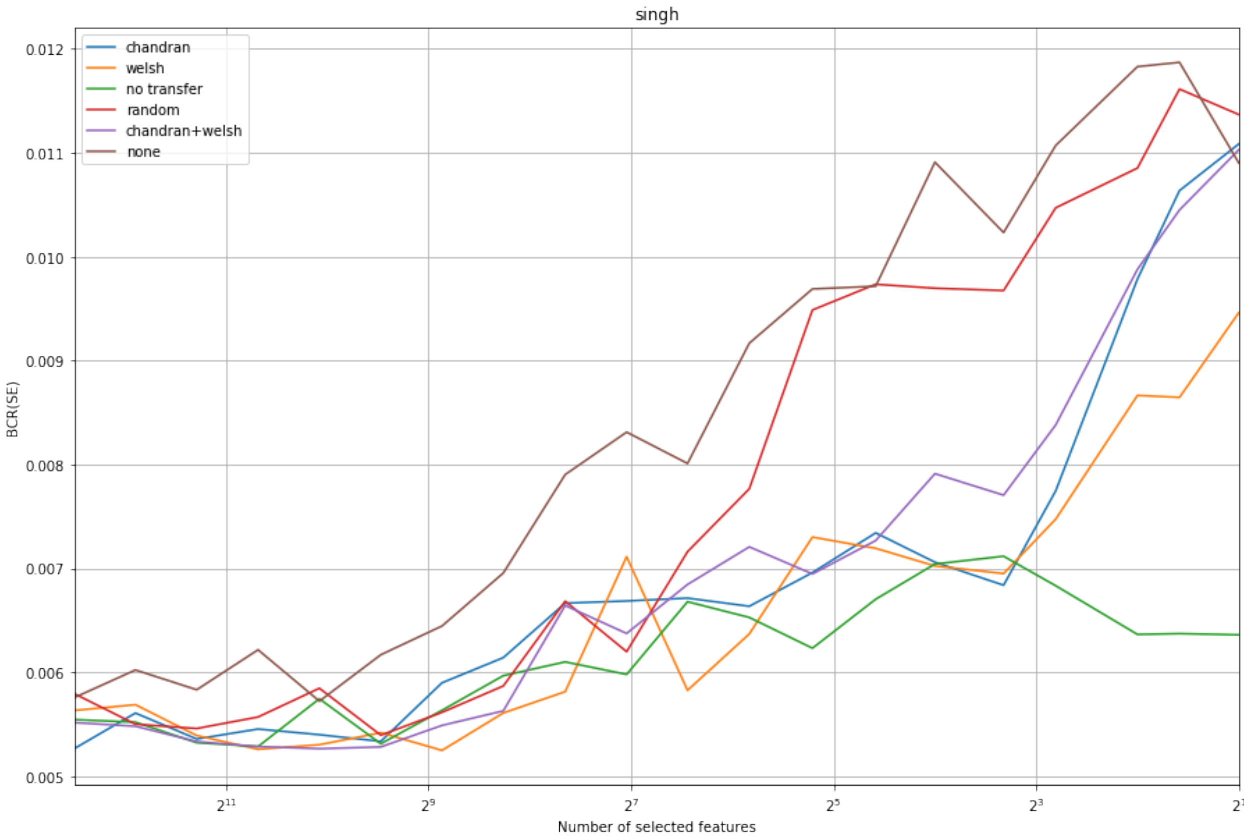
Standard error is relatively high and could weaken in a high amount the conclusions ot this statistical experiment. It's necessary to increase the iteration number to see if we can reduce this metric.

Script 1.3.6 (python)

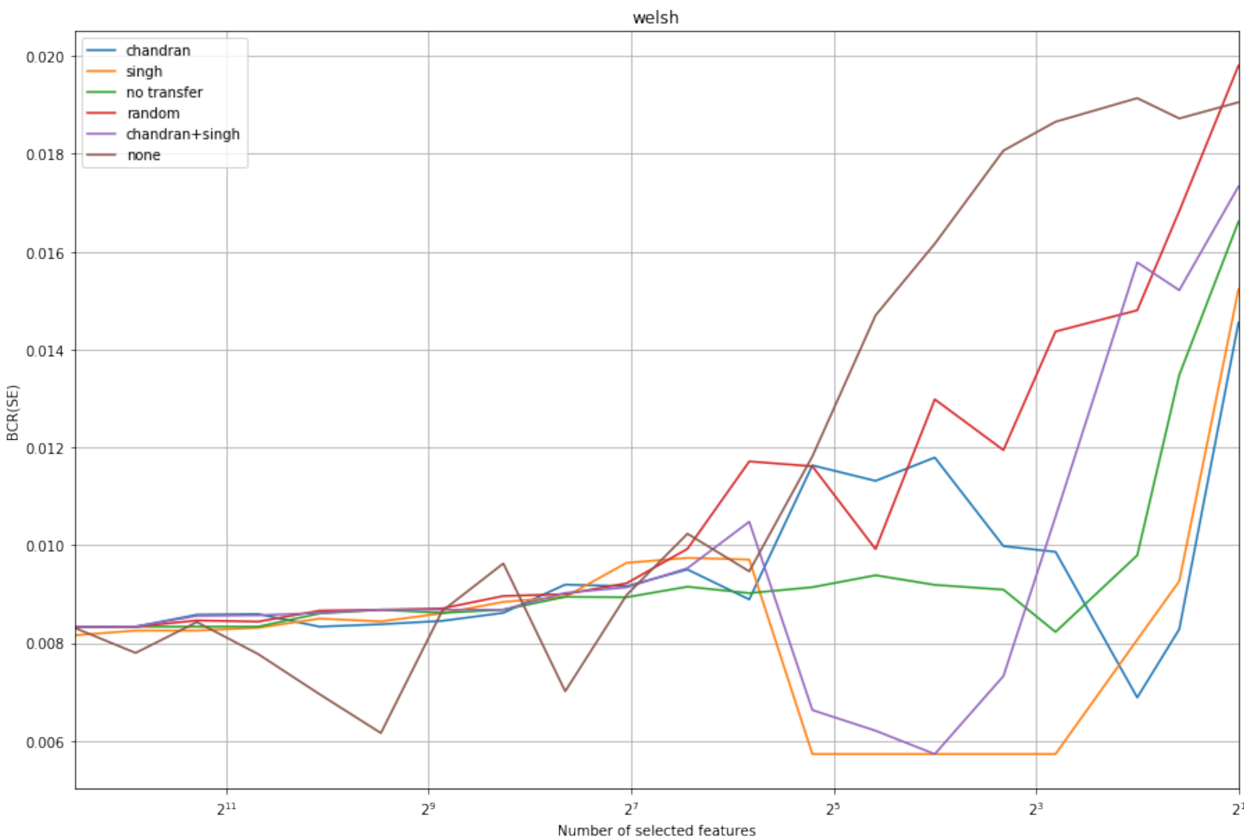
```python
idx_target = 0
df_bcr_mean = pd.DataFrame(df_bcr.groupby(['target', 'source', 'num features'])['BCR'].sem()).reset_index()
for idx_target in [0,1,2]:
    target = SAMPLE_NAMES[idx_target]
    df_target = df_bcr_mean.loc[df_bcr_mean['target'] == target]
    plt.figure(figsize=(15,10))
    plt.xscale('log', basex=2)
    for idx_source in [0,1,2,3,4, DUAL_TRANSFER_IDX + idx_target, 8]:
        #if idx_source in FILTER_SOURCES and idx_source!= idx_target:
```

```
        if idx_source!= idx_target:
            label = SAMPLE_NAMES[idx_source]
            df_source = df_target[df_target['source'] == label]
            plt.xlim(max(df_source['num features']), min(df_source['num features']))
            plt.plot(df_source['num features'], df_source['BCR'], label=label)

    plt.title(target)
    plt.xlabel("Number of selected features")
    #plt.xlim(100,400)
    #plt.xticks(df_source['num features'])
    plt.ylabel("BCR(SE)")
    plt.legend(loc = "best")
    plt.grid()
    plt.show()
```





singh
chandran
welsh
no transfer
random
chandran+welsh
none
0.012
0.011
0.010
0.009
0.008
0.007
0.006
0.005
BCR(SE)
2^{11}
2^{9}
2^{7}
2^{5}
2^{3}
2^{1}
Number of selected features



1.3.7 Calculate stability

Script 1.3.7 (python)

```python
stability = []
for idx_target in FILTER_TARGETS:
    target = SAMPLE_NAMES[idx_target]
    df_target = df_bcr.loc[df_bcr['target'] == target]
    for idx_source in [0,1,2,3,4, DUAL_TRANSFER_IDX + idx_target, 8]:
        if idx_source!= idx_target:
            source = SAMPLE_NAMES[idx_source]
            df_source = df_target[df_target['source'] == source]
            n_features = np.unique(df_source['num features'])
            #print(n_features)
            for num_features in n_features:
                df_num_features = df_source[df_source['num features'] == num_features]
                # Calculate stability
                s = num_features
                s2 = s**2
                n = 12598
                s2_n = s2/n
                den = s - s2_n
```

```python
                list_S = list(df_num_features['S'])
                stab = 0
                count = 0
                k = len(list_S)
                for i in range(k):
                    for j in range(i+1, k):
                        Si_Sj = np.intersect1d(list_S[i], list_S[j])
                        stab += (len(Si_Sj) - s2_n) / den
                        count += 1
                stability.append([target, source, num_features, stab/count])
                #print(1/count, 2/(k*(k-1)), stability[-1], 2*stab/(k*(k-1)))

df_stab = pd.DataFrame(stability, columns=['target', 'source', 'num features', 'stability'])
df_stab.head()
```

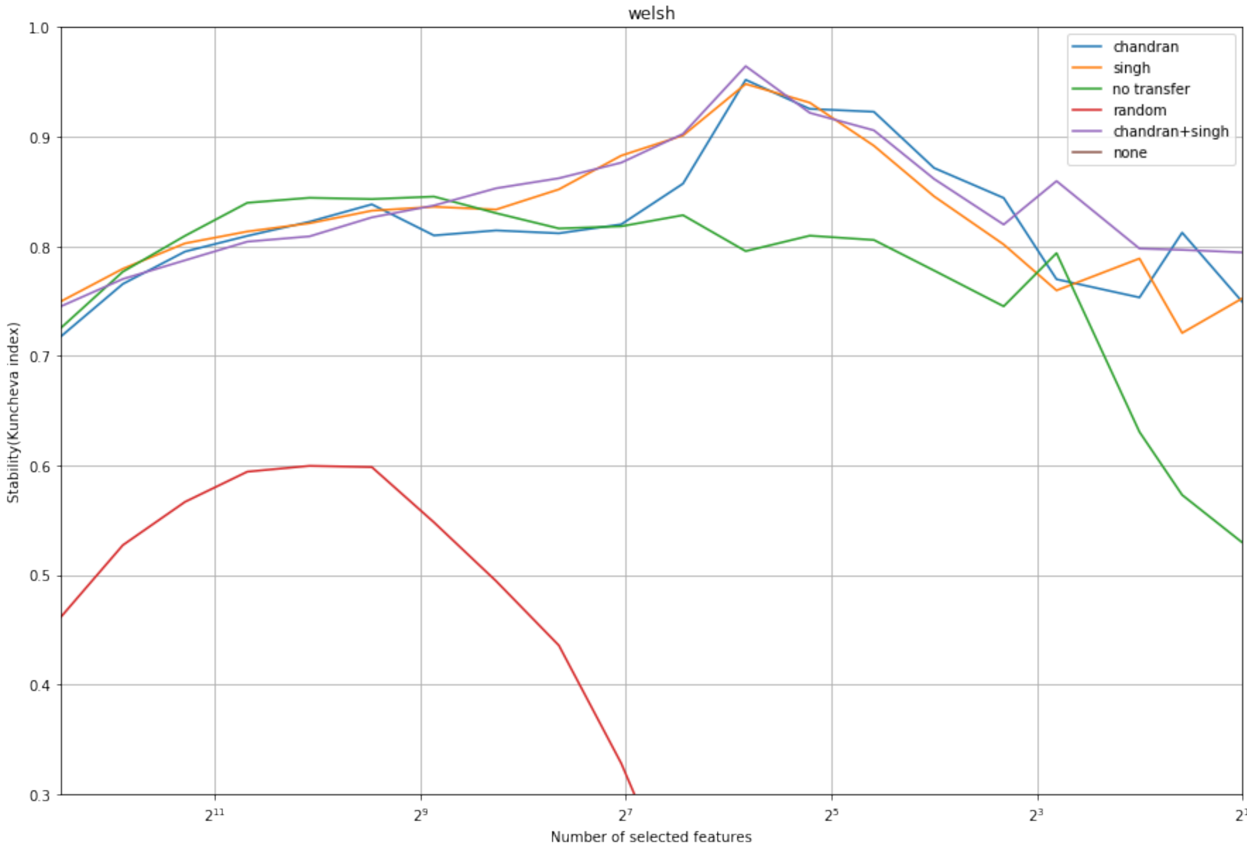
Display output

```
     target source  num features  stability
0  chandran  singh             2   0.334769
1  chandran  singh             3   0.370537
2  chandran  singh             4   0.454563
3  chandran  singh             7   0.590174
4  chandran  singh            10   0.726014
```

1.3.8 Plot stability

Script 1.3.8 (python)

```python
idx_target = 0
for idx_target in FILTER_TARGETS:
    target = SAMPLE_NAMES[idx_target]
    df_target = df_stab.loc[df_stab['target'] == target]
    plt.figure(figsize=(15,10))
    plt.xscale('log', basex=2)
    for idx_source in [0,1,2,3,4, DUAL_TRANSFER_IDX + idx_target, 8]:
        #if idx_source in FILTER_SOURCES and idx_source!= idx_target:
        if idx_source!= idx_target:
            label = SAMPLE_NAMES[idx_source]
            df_source = df_target[df_target['source'] == label]
            plt.xlim(max(df_source['num features']), min(df_source['num features']))
            plt.plot(df_source['num features'], df_source['stability'], label=label)

    plt.title(target)
    plt.xlabel("Number of selected features")
    plt.ylim(0.3, 1)
    #plt.xticks(df_source['num features'])
    plt.ylabel("Stability(Kuncheva index)")
    plt.legend(loc = "best")
    plt.grid()
    plt.show()
```



1.3.9 Impact of B

BCR

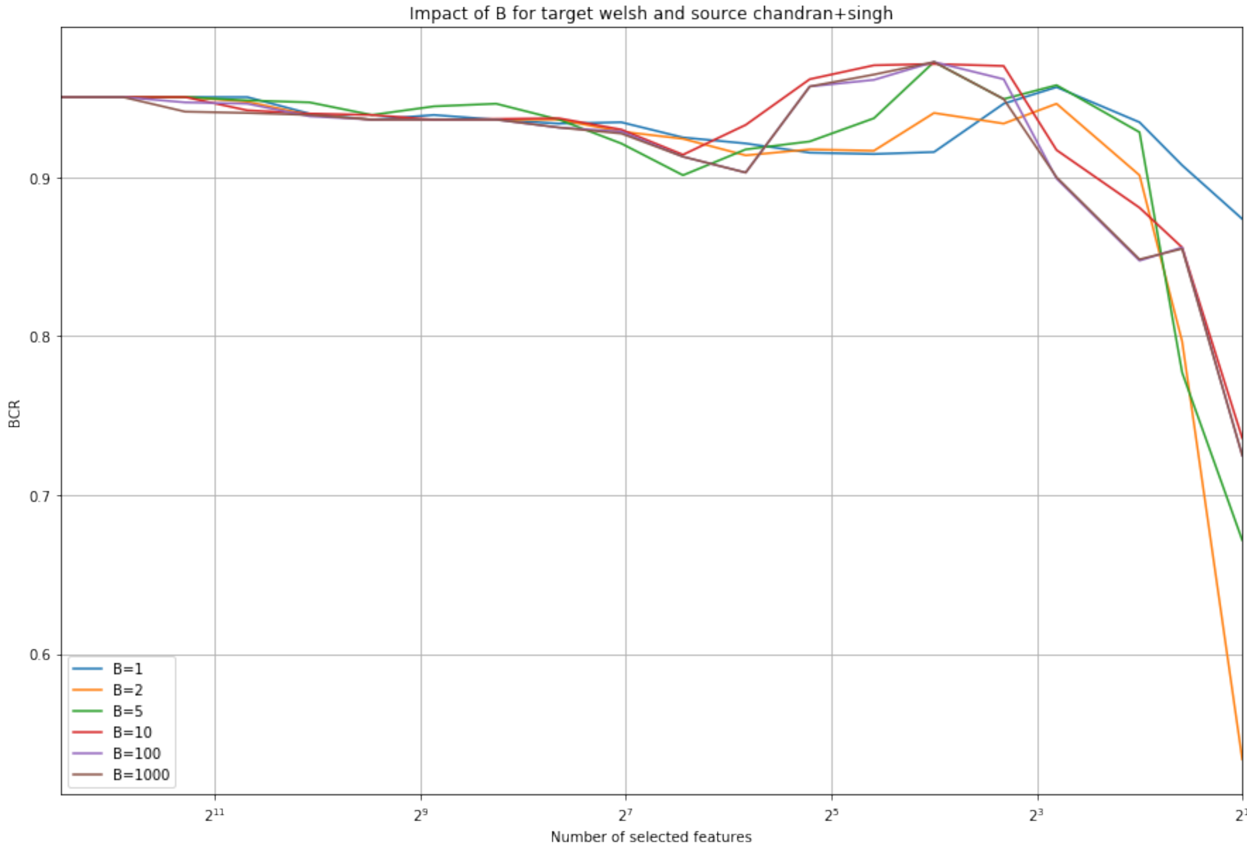
Script 1.3.9 (python)

```python
FILTER_TARGETS = [2] #welsh
#features_to_select = np.unique(np.logspace(2, 12.5, num=50, endpoint=True, base=2.0,
↪  dtype=int))
bcr_list = []
B_values = [1,2,5,10,100,1000]
for g_B in B_values:
    for g_k in range(0,200):
        for idx_target in FILTER_TARGETS:
            #print("TARGET", SAMPLE_NAMES[idx_target])
            X_train_scaled_target, X_test_scaled_target, y_train_target, y_test_target =\
            get_target_data_sets(df_samples_norm, idx_target)
            for idx_source in [DUAL_TRANSFER_IDX + idx_target]:
                print("k", g_k, "TARGET", SAMPLE_NAMES[idx_target], "SOURCE",
                ↪  SAMPLE_NAMES[idx_source])
                for features_selected in features_to_select:
                    #print("Features",features_selected)
```

```
                    bcr, ranking_selected = compute_transfer(X_train_scaled_target, X_test_scaled_target, y_train_target, y_test_target,\
                                            idx_source=idx_source, num_features_selected=features_selected)
                    bcr_list.append([g_B, features_selected, bcr, ranking_selected])
                    if VERBOSE: print("Target", idx_target, "Source", idx_source, "#Features",\
                                      features_selected, "BCR", bcr)

df_bcr_B = pd.DataFrame(bcr_list, columns=['B', 'num features', 'BCR', 'S'])
df_bcr_B.head()
```

Script 1.3.10 (python)

```
idx_target = 2
df_bcr_mean = pd.DataFrame(df_bcr_B.groupby(['B', 'num features'])['BCR'].mean()).reset_index()

target = SAMPLE_NAMES[2]
source = SAMPLE_NAMES[DUAL_TRANSFER_IDX + idx_target]
plt.figure(figsize=(15,10))
plt.xscale('log', basex=2)
for idx_B in B_values:
    df_B = df_bcr_mean.loc[df_bcr_mean['B'] == idx_B]
    plt.xlim(max(df_B['num features']), min(df_B['num features']))
    plt.plot(df_B['num features'], df_B['BCR'], label='B=' + str(idx_B))
plt.title("Impact of B for target " + target + " and source " + source)
plt.xlabel("Number of selected features")
#plt.xlim(100,400)
#plt.xticks(df_source['num features'])
plt.ylabel("BCR")
plt.legend(loc = "best")
plt.grid()
plt.show()
```



Stability

Script 1.3.11 (python)

```
stability = []
for idx_B in B_values:
    df_B = df_bcr_B.loc[df_bcr_B['B'] == idx_B]
    n_features = np.unique(df_bcr['num features'])
    #print(n_features)
    for num_features in n_features:
        df_num_features = df_B[df_B['num features'] == num_features]
        # Calculate stability
        s = num_features
        s2 = s**2
        n = 12598
        s2_n = s2/n
        den = s - s2_n
        list_S = list(df_num_features['S'])
        stab = 0
        count = 0
        k = len(list_S)
        for i in range(k):
```

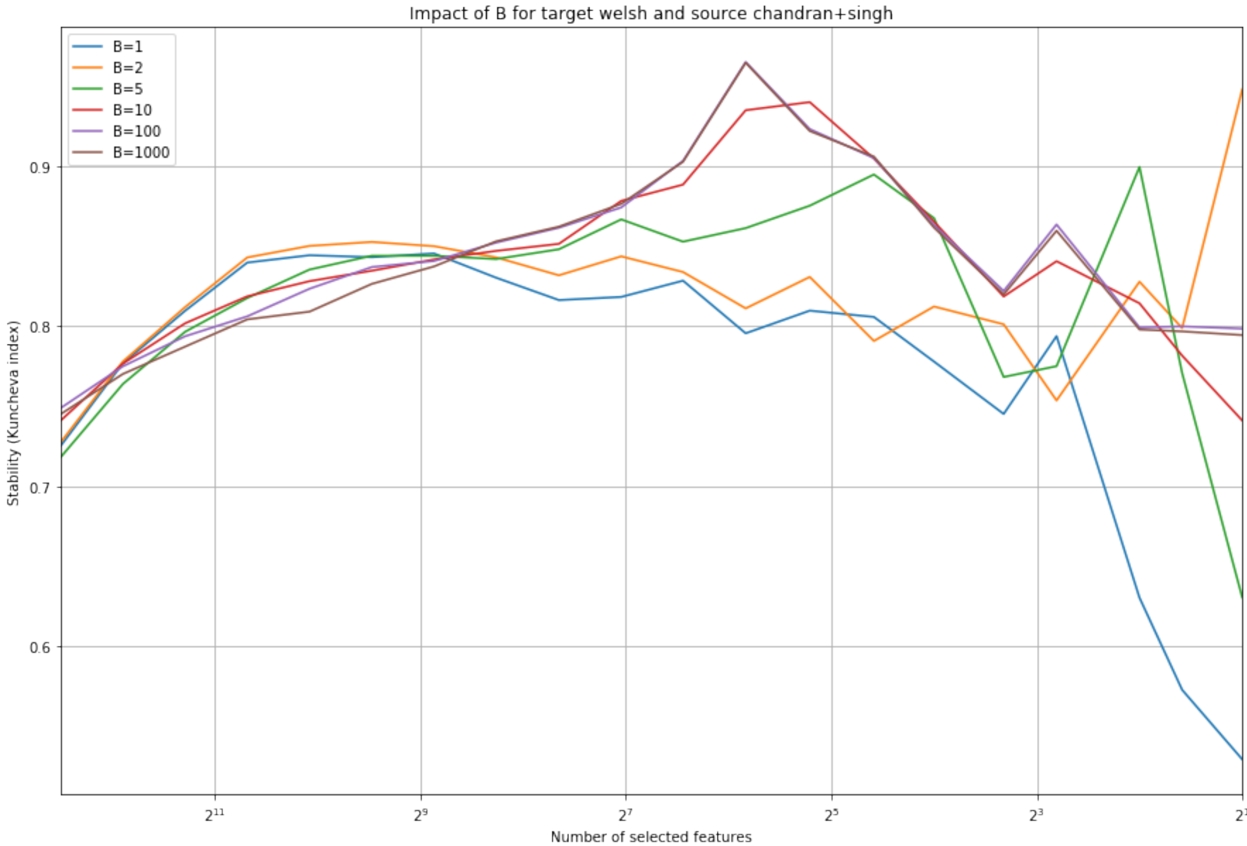
```python
            for j in range(i+1, k):
                Si_Sj = np.intersect1d(list_S[i], list_S[j])
                stab += (len(Si_Sj) - s2_n) / den
                count += 1
        stability.append([idx_B, num_features, stab/count])
        #print(1/count, 2/(k*(k-1)), stability[-1], 2*stab/(k*(k-1)))

df_stab_B = pd.DataFrame(stability, columns=['B', 'num features', 'stability'])
df_stab_B.head()
```

Display output

	B	num features	stability
0	1	2	0.529699
1	1	3	0.573081
2	1	4	0.630561
3	1	7	0.793791
4	1	10	0.745220

Script 1.3.12 (python)

```python
target = SAMPLE_NAMES[idx_target]
source = SAMPLE_NAMES[DUAL_TRANSFER_IDX + idx_target]
plt.figure(figsize=(15,10))
plt.xscale('log', basex=2)
for idx_B in B_values:
    df_B = df_stab_B.loc[df_stab_B['B'] == idx_B]
    plt.xlim(max(df_B['num features']), min(df_B['num features']))
    plt.plot(df_B['num features'], df_B['stability'], label='B=' + str(idx_B))
plt.title("Impact of B for target " + target + " and source " + source)
plt.xlabel("Number of selected features")
#plt.xlim(100,400)
#plt.xticks(df_source['num features'])
plt.ylabel("Stability (Kuncheva index)")
plt.legend(loc = "best")
plt.grid()
plt.show()
```



Impact of B for target welsh and source chandran+singh
B=1
B=2
B=5
B=10
B=100
B=1000
Stability (Kuncheva index)
0.6
0.7
0.8
0.9
2^11
2^9
2^7
2^5
2^3
2^1
Number of selected features