

```
[28]: import sys
sys.path.insert(0, '/Users/jussakor/.local/lib/python3.9/site-packages')
sys.path.remove('/scratch/project_2003855/jupyter_scripts/numpy-1.21.0-py3.9-nozmq32')
sys.path.remove('/Users/jussakor/.local/lib/python3.9/site-packages')
!reset -f
```

Table of Contents

- Introduction
- Load and normalize the data
- Run PLS-analysis
- Evaluate the PLS-analysis results
- Confounding Variable Analysis
- Significant Latent Component Analysis
 - Bootstrapping results
 - Driving imaging features
 - Driving behavioral features

Introduction

Psychopathy is an antisocial personality disorder that is highly correlated with crime and violence. Psychopathy Check List Revised (PCL-R) provides a clinical assessment of the degree of psychopathy that an individual possesses. Specific scoring criteria rate twenty separate items on a three-point scale (0, 1, 2) to determine the extent to which they apply to a given individual. In this analysis we do Partial Least Squares (PLS) analysis on fMRI images of PCL-R assessed forensic patients, to see if there exists reliable biomarkers that correlate with the subscores of the PCL-R. Sample size is 51. As preprocessing, grey matter (GM) images are segmented from the MRI images with SPM software. Then, regional volumes are calculated from the GM images with masks provided also by the SPM software. These regional volumes are then normalized with total GM volume, so that we analyze volumes relative to individuals total GM volume instead of analyzing absolute volumes.

PLS aims to find latent components (linear combinations) from both volume features X and behavior measures Y, that maximally correlate. This is achieved by doing Singular-Value-Decomposition (SVD) on the correlation matrix R which is calculated from normalized X (X0) and normalized Y (Y0) as R = transpose(Y0) * X0.

Load and normalize the data

```
[29]: import numpy as np
import nibabel as nib

# Load data
metadata = pd.read_csv('/scratch/project_2003855/data/NIWA/METADATA/PCL_R.csv')
img_size = [121,145,121]
n_samp = 51
voxels = np.zeros((n_samp, img_size))

for filepath, i in zip(metadata[["GM_filepath_csc"]], range(n_samp)):
    # Load 3D image
    fp = filepath.replace("csmpl", "nmp1") # unsmoothed
    img_nifti = nib.load(fp)
    # Get voxel values
    img = img_nifti.get_fdata()
    # Vectorize to 1D and store in X
    voxels[i, :] = img.flatten()

# NORMALIZATION!!! this is very critical for the results
from sklearn.preprocessing import normalize
voxels = normalize(voxels, norm='l1', axis=1) # default is row-wise L2-normalization

[30]: from scipy.ndimage import ndimage
import nibabel as nib
import numpy as np
import matplotlib.pyplot as plt
from ipynbwidgets import interact, interactive, fixed, interact_manual
from matplotlib.colors import LogNorm
from scipy.ndimage import zoom
import matplotlib.pyplot as plt
from nibabel.niimg import Nifti1Image
# Load the SPM atlas to get masks for different brain regions
atlas = nib.load('/scratch/project_2003855/jupyter_scripts/atlasData/labels_Neuroanatomical.nii')
# Get voxel values
atlas = atlas.get_fdata()
# Vectorize 3D image
temp = atlas.flatten()
region_id = np.unique(atlas[1:]) # 0 is background
# Get region names from separate xml file
tree = ET.parse('/scratch/project_2003855/jupyter_scripts/atlasData/ROI1labels.xml')
root = tree.getroot()
region_names = [root[i][1][1].text for i in range(n_region)]
Regional_Volumes = pd.DataFrame(data=np.zeros((51, n_region)), columns=region_names)

for region_id, i in zip(region_id, range(n_region)):
    Regional_Volumes.loc[:, i] = np.sum(voxels[:, temp==region_id], axis=1)

plot_atlas = 0
if plot_atlas:
    # Examples of how areas are labeled in atlas (first is left, and then right)
    # examples:
    # atlas==31 | atlas==32
    # orbitofrontal cortex:
    # atlas==104 | atlas==105 ...
    # atlas==145 | atlas==147
    # anterior cingulate gyrus:
    # atlas==108 | atlas==109
    # hippocampus:
    # atlas==47 | atlas==48
    region = 32
    wholemask = atlas.copy()
    wholemask[wholemask != region] = 0

    def explore_3d_image(layer):
        plt.figure(figsize=(10, 10))
        im = ndimage.rotate(atlas[:, :, layer], -90)
        mask = ndimage.rotate(wholemask[:, :, layer], -90)
        plt.imshow(im, cmap='gray', vmin=0, vmax=255)
        plt.imshow(mask, cmap='coolwarm', vmin=-1, vmax=1, alpha=0.5)
        plt.axis('off')
        plt.colorbar(fraction=0.046, pad=0.04)
        return layer
    interact(explore_3d_image, layer=(0, 120))

Fill the missing subscores according to total score (even distribution)
```

```
[31]: Y = metadata.iloc[:, 38:50]
for i in range(Y.iloc[0, :].isna().sum()):
    for row in np.where(Y.isna().any(axis=1))[0]:
        #print(row)
        # Calculate missing part of the total score
        m = Y.iloc[row, 0] - np.nansum(Y.iloc[row, 1:])
        missing = np.where(Y.iloc[row, 1:].isna())
        # Divide the missing part equally to Nans
        fillval = np.ceil(m / len(missing))
        Y.iloc[row, missing] = fillval

#from pandas import DataFrame
DataFrame(np.array([Y["PCL_R_tot"], np.sum(Y.iloc[:, 1:], axis=1), Y["PCL_R_tot"] - np.sum(Y.iloc[:, 1:], axis=1)]), Y)
```

```
[32]: x = Regional_Volumes
# Remove total score
x = x.iloc[:, 1:]
subscore_names = Y.columns
print('Shape of X:', np.shape(x))
print('Shape of Y:', np.shape(Y))
print('Behaviors:', subscore_names)

Shape of X: (51, 136)
Shape of Y: (51, 120)
Behaviors: Index([1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50], dtype='object', length=50)
```

Or load the data as numpy arrays:

```
[32]: import numpy as np
from saved = True

if from saved:
    x = np.genfromtxt('/scratch/project_2003855/jupyter_scripts/Brain.csv', delimiter=',')
    y = np.genfromtxt('/scratch/project_2003855/jupyter_scripts/numpyData/RegionalVolumesTotalScore.csv', delimiter=',', skip_header=True)
    y1 = np.genfromtxt('/scratch/project_2003855/jupyter_scripts/numpyData/F1.csv', delimiter=',', skip_header=True) # Factor 1
    y2 = np.genfromtxt('/scratch/project_2003855/jupyter_scripts/numpyData/F2.csv', delimiter=',', skip_header=True) # Factor 2
    y3 = np.genfromtxt('/scratch/project_2003855/jupyter_scripts/numpyData/CofoundingVariables.csv') # possibly cofounding variables
    covars_bin = pd.get_dummies(covars)
    x = np.concatenate((x, covars_bin), axis=1)
    y = np.concatenate((y, y1, y2, y3), axis=1)
    y1 = y2
    y = y2
    print(y.shape)

# Load the subscore labels names separately through Pandas:
import pandas as pd
from ipynbwidgets import interact, display, HTML
temp = pd.read_csv('/scratch/project_2003855/jupyter_scripts/numpyData/F1.csv')
temp2 = pd.read_csv('/scratch/project_2003855/jupyter_scripts/numpyData/F2.csv')
subscore_names = np.concatenate([["F1", "F2"], list(temp.columns), list(temp2.columns)], axis=0)
covars_bin_names = np.concatenate([["F1", "F2"], list(temp.columns), list(temp2.columns), list(temp2.columns), list(temp2.columns), list(temp2.columns)], axis=0)
covars_bin_names = np.concatenate([["Factor 1 total", "Factor 2 total"], list(temp2.columns), list(temp2.columns)], axis=0)
subscore_names = np.concatenate([["Factor 1 labels", "Factor 2 labels"], list(temp2.columns), list(temp2.columns)], axis=0)
else:
    temp = pd.read_csv('/scratch/project_2003855/jupyter_scripts/numpyData/F1.csv')
    temp2 = pd.read_csv('/scratch/project_2003855/jupyter_scripts/numpyData/F2.csv')
    F1 = np.sum(temp.columns, axis=1)
    F2 = np.sum(temp2.columns, axis=1)
    F2 = np.concatenate((F1, F2), axis=1)
    x = x.to_numpy()
    y = y.to_numpy()
    x = x.to_numpy()
    y = y.to_numpy()

(51, 136)
(51, 120)
```

	Factor 1 labels	Factor 2 labels
0	1. Glibness/Superficial Charm	3. Need for Stimulation/Proneness to Boredom
1	2. Grandiose Sense of Self Worth	9. Parasitic Lifestyle
2	4. Pathological Lying	10. Poor Behavioral Controls
3	5. Cunning/Manipulative	11. Promiscuous Sexual Behavior
4	6. Lack of Remorse of Guilt	13. Lack of Realistic, Long-term Goals
5	7. Shallow Affect	14. Impulsivity
6	8. Callous/Lack of Empathy	15. Irresponsibility
7	16. Failure to Accept Responsibility for Own Actions	18. Juvenile Delinquency
8	17. Many Short-term Marital Relationships	19. Revocation of Conditional Release
9	20. Criminal Versatility	19. Revocation of Conditional Release

Normalize the input features X and output behaviors Y with standard scaling. Alternatively we could just not do this feature wise normalization, but then the differences in large regions would dominate.

```
[34]: from sklearn import preprocessing
scalerX = preprocessing.StandardScaler().fit(X)
X0 = scalerX.transform(X)
scalerY = preprocessing.StandardScaler().fit(Y)
Y0 = scalerY.transform(Y)
```

Or then we do the normalization scanner-wise in order to correct the scanner effect (not working):

```
[35]: """
from sklearn import preprocessing
# possibly cofounding variables
if from saved:
    covars = pd.read_csv('/scratch/project_2003855/jupyter_scripts/numpyData/CofoundingVariables.csv') #possibly cofounding variables
    covars.columns = ["SEX", "ManufacturerModelName", "AGE"]
else:
    covars = metadata[["AGE", "ManufacturerModelName"]]
    # not legit, we don't know the ages of Niwa images
    covars.AGE = covars.AGE.fillna(30)
    # the Niwa images are scanned with Siemens scanner
    covars.ManufacturerModelName = covars.ManufacturerModelName.fillna("Siemens")

grouping = 0

if grouping:
    scanners = covars["ManufacturerModelName"]
    Xdf = pd.DataFrame(data=X)
    Xdf["group"] = scanners
    Xdf = Xdf.groupby("group").transform(lambda x: (x - x.mean()) / x.std())
    XB = Xdf.to_numpy()
    Ydf = pd.DataFrame(data=Y)
    Ydf["group"] = scanners
    Ydf = Ydf.groupby("group").transform(lambda x: (x - x.mean()))
    YB = Ydf.to_numpy()
    """

Out[35]: ["from sklearn import preprocessing\npossibly cofounding variables\nif from saved:\n    covars = pd.read_csv('/scratch/project_2003855/jupyter_scripts/numpyData/CofoundingVariables.csv')\n    covars.columns = [\"SEX\", \"ManufacturerModelName\", \"AGE\"]\nelse:\n    covars = metadata[\"AGE\", \"ManufacturerModelName\"]\n    # not legit, we don't know the ages of Niwa images\n    covars.AGE = covars.AGE.fillna(30)\n    # the Niwa images are scanned with Siemens scanner\n    covars.ManufacturerModelName = covars.ManufacturerModelName.fillna(\"Siemens\")\n\nXdf = pd.DataFrame(data=X)\nXdf[\"group\"] = scanners\nXdf = Xdf.groupby(\"group\").transform(lambda x: (x - x.mean()) / x.std())\nXB = Xdf.to_numpy()\n\nYdf = pd.DataFrame(data=Y)\nYdf[\"group\"] = scanners\nYdf = Ydf.groupby(\"group\").transform(lambda x: (x - x.mean()))\nYB = Ydf.to_numpy()\n"]
```

Run the PLS-analysis

```
[36]: # run the analysis and look at the results structure
from pys import behavioral_pls
# groupid option takes the cofounding scanner effect into consideration
grouped = 0
if grouped:
    if from saved:
        covars = pd.read_csv('/scratch/project_2003855/jupyter_scripts/numpyData/CofoundingVariables.csv') #possibly cofounding variables
        covars.columns = ["SEX", "ManufacturerModelName", "AGE"]
    else:
        covars = metadata[["AGE", "ManufacturerModelName"]]
        # not legit, we don't know the ages of Niwa images
        covars.AGE = covars.AGE.fillna(30)
        # the Niwa images are scanned with Siemens scanner
        covars.ManufacturerModelName = covars.ManufacturerModelName.fillna("Siemens")
    scanners = covars["ManufacturerModelName"]
    Xdf = pd.DataFrame(data=X)
    Xdf["group"] = scanners
    Xdf = Xdf.sort_values("group")
    Xdf = Xdf.drop("group", axis=1)
    XB = Xdf.to_numpy()
    Ydf = pd.DataFrame(data=Y)
    Ydf = Ydf.sort_values("group")
    groups = Ydf.groupby("group").size().values
    Ydf = Ydf.drop("group", axis=1)
    YB = Ydf.to_numpy()

print(groups)
bpls = behavioral_pls(XB, YB, groups=groups, n_procs='max', verbose=False)
else:
    bpls = behavioral_pls(XB, YB, n_procs='max', test_split=0, test_size=0, verbose=False, seed=1234)
bpls
```

Out[36]: PLSResults(x_weights, y_weights, x_scores, y_scores, y_loadings, singulars, varexp, perares, bootres, inputs)

Evaluate PLS-analysis results

Let us how much of the covariance (variance of R) is captured by our latent components:

```
[37]: bpls.varexp

array([0.52234592, 0.09529774, 0.07408434, 0.0509722, 0.04730812,
       0.0393069, 0.02748094, 0.02901693, 0.02030937, 0.01026424,
       0.0157017, 0.0184114, 0.00949029, 0.0086271, 0.00702415,
       0.00553924, 0.00539246, 0.00369562, 0.0026619, 0.0016451])
```

Permutation testing over singular values: Which components are significant?

During the analysis, permutation testing is done in order to evaluate whether the signal is different from noise. This is done through shuffling the labels, doing the PLS analysis again and seeing how much variance is captured when the newly created latent components. This is done 5000 times to create a noise distribution, from which the p-value is then calculated for the original values of the captured variance.

```
[38]: perares = bpls.get("perares")
perares.get("p01")

array([1.99960000e-04, 6.99898020e-03, 4.13173370e-01, 3.32133570e-01,
       2.72745450e-01, 7.74457310e-01, 3.00434320e-01, 5.71485760e-01,
       9.40811380e-01, 9.88024000e-01, 9.76847130e-01, 9.70685870e-01,
       9.52089180e-01, 9.73050360e-01, 9.06200400e-02, 9.06200400e-02,
       1.00000000e+00, 1.00000000e+00, 9.99800040e-01, 1.00000000e+00])
```

After correcting the p-values for multiple comparison (feature size 136), we are left with 1 significant latent component (1st latent component).

Posthoc t-tests on PLS scores: Are components differently expressed by groups?

We do posthoc t-tests on x-scores between psychopaths (total score > 25) and non-psychopaths (total score <= 25). The significance of the results is questionable since the components were already discovered using subscores.

```
[39]: from scipy import stats
PCL_R_tot_score = np.sum(Y, axis=1)
is_psycho = (PCL_R_tot_score > 25)
stats.ttest_ind(bpls.x_scores[is_psycho==1], bpls.x_scores[is_psycho==0], equal_var=False)
```

Out[39]: Ttest_indResult(statistic=-3.8161014317433555, pvalue=0.00042698122636556)

Significant Latent Component Analysis

Lets check the Pearson correlation between the x-scores (points in the volume coordinate space reflected onto the imaging latent component) and the y-scores (points in the behavior measure space reflected onto the respective behavioral latent components)

```
[40]: from scipy.stats import pearsonr
lc = 0
pearsonr(bpls.x_scores[:,lc], bpls.y_scores[:,lc])[0]

Out[40]: 0.747879356555557
```

Bootstrap estimation of saliences' standard errors: Which PLS loadings are stable?

adjustment (usually distorted by choice of standard/imaging saliences) can be considered as the coefficients for the original imaging variables to construct the latent component. To estimate the standard errors of the saliences, we create bootstrap samples which are obtained by sampling with replacement from X. A salience standard error is then estimated as the standard error of the saliences from a large number of these bootstrap samples (5000 in our case). The ratios (salience / standard error of the saliences) are then taken to be a Z-score. Therefore when they are larger than 2 the corresponding saliences are considered significantly stable. Stable saliences determine which imaging variables show reliable responses to the behavioral measures (across the population, not dependent on outliers).

```
[41]: import matplotlib.pyplot as plt
plt.hist(bpls.bootres.x_weights_normed[:,lc])
plt.title('Histogram of z-scores of saliences')
plt.show()

Histogram of z-scores of saliences
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