

log_model

April 27, 2023

```
[1]: import ants
import glob
import os
from sklearn.decomposition import PCA
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression
from multiprocessing import Pool
import gc

import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

0.1 Read in the data

All data is in one folder, so we need to split the files into white matter and gray matter

```
[2]: def get_ordered_files(directory, prefix):

    # Get a list of all files in the directory
    all_files = os.listdir(directory)

    # Filter files that start with prefix
    files = [f for f in all_files if f.startswith(prefix)]

    # Filter again for wm and gm
    gm_files = [f for f in files if f.endswith('-gm.nii.gz')]
    wm_files = [f for f in files if f.endswith('-wm.nii.gz')]

    # Sort the files list
    sorted_gm_files = sorted(gm_files)
    sorted_wm_files = sorted(wm_files)

    return sorted_gm_files, sorted_wm_files
```

```
[3]: data_path = '/scratch/users/neuroimage/conda/data'
img_path = os.path.join(data_path, 'preprocessed/imgsss')

smt_files_gm, smt_files_wm = get_ordered_files(img_path, "smt")
snmt_files_gm, snmt_files_wm = get_ordered_files(img_path, "snmt")
nsmt_files_gm, nsmt_files_wm = get_ordered_files(img_path, "nsmt")
```

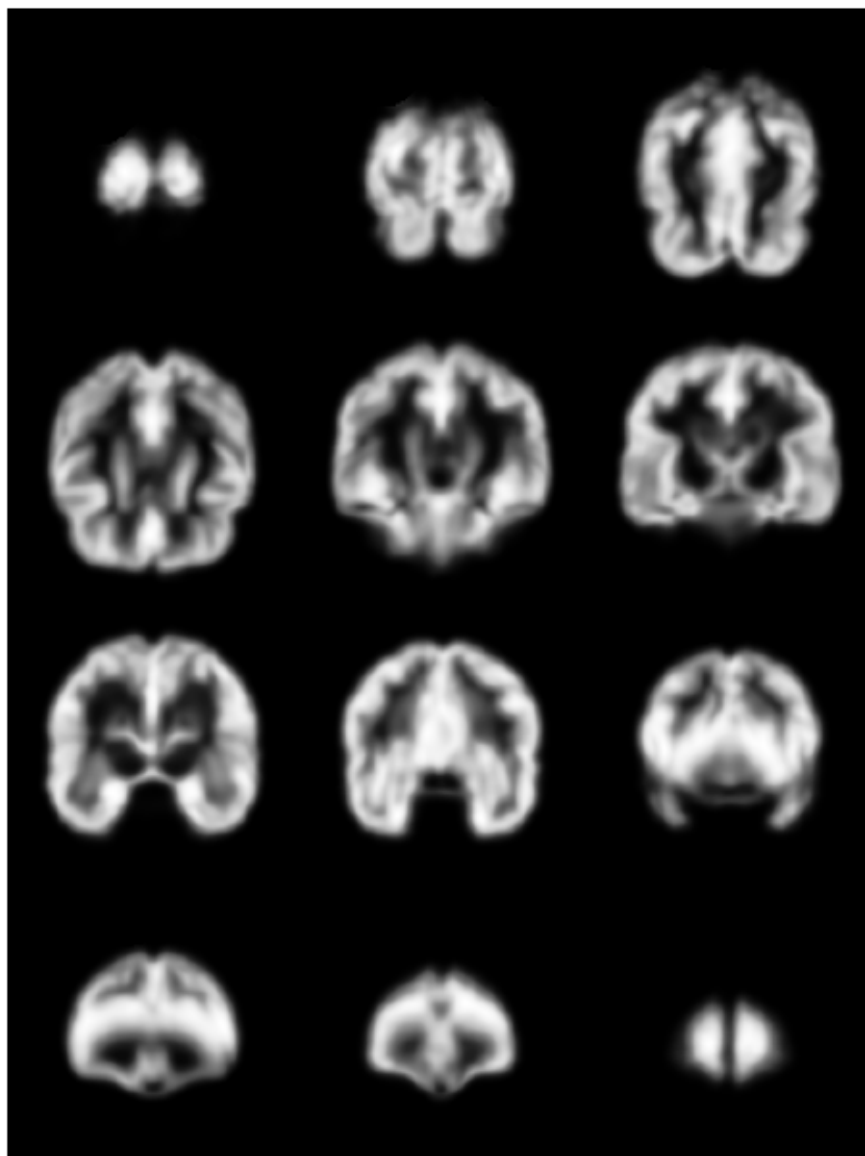
```
[4]: print(smt_files_gm[0], smt_files_wm[0])
print(snmt_files_gm[0], snmt_files_wm[0])
print(nsmt_files_gm[0], nsmt_files_wm[0])
```

```
smt-002_S_0413-I118675-gm.nii.gz smt-002_S_0413-I118675-wm.nii.gz
snmt-002_S_0413-I118675-gm.nii.gz snmt-002_S_0413-I118675-wm.nii.gz
nsmt-002_S_0413-I118675-gm.nii.gz nsmt-002_S_0413-I118675-wm.nii.gz
```

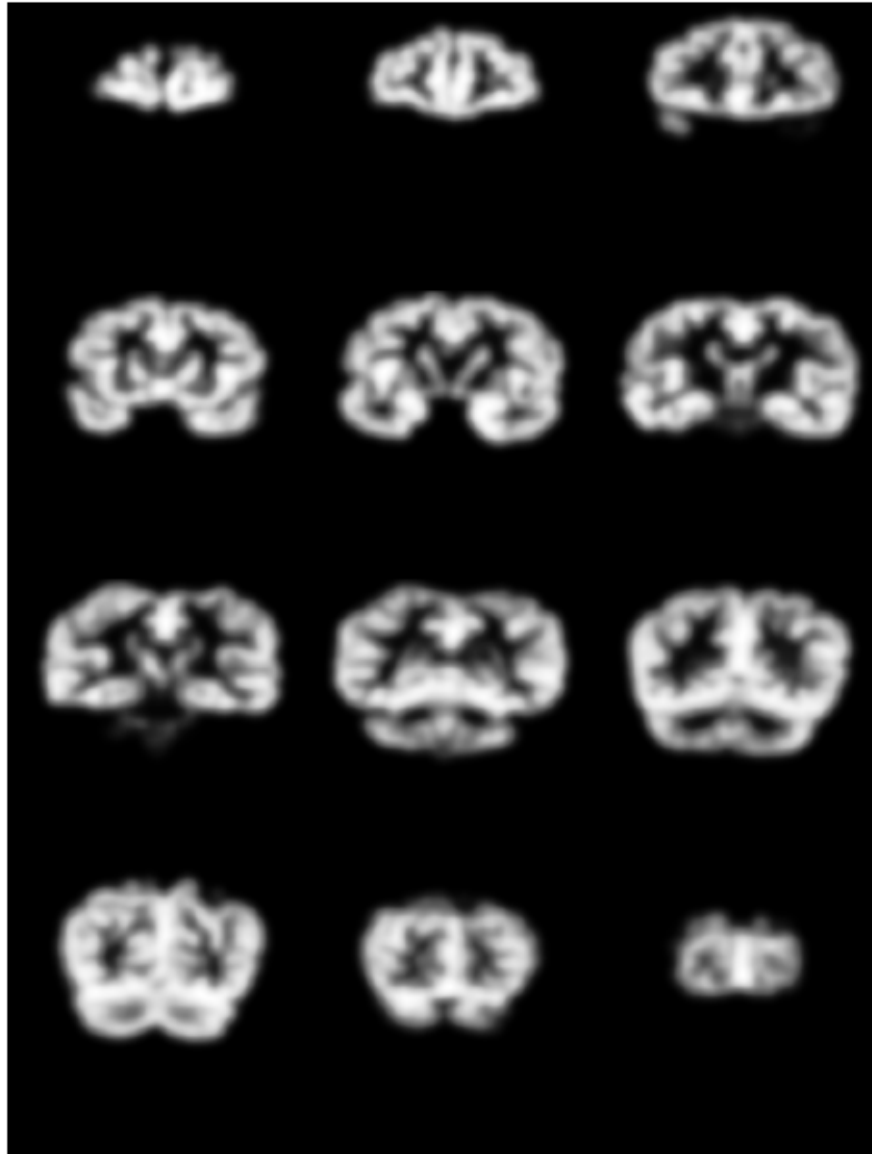
Visualizing the difference in smooth mapped to template, smooth but not mapped to template and not smooth but mapped to template

```
[5]: print("SMT")
ants.plot(os.path.join(img_path, smt_files_gm[1]),axis=1)
print("SNMT")
ants.plot(os.path.join(img_path, snmt_files_gm[0]),axis=1)
print("NSMT")
ants.plot(os.path.join(img_path, nsmt_files_gm[0]),axis=1)
print("SMT")
ants.plot(os.path.join(img_path, smt_files_wm[0]),axis=1)
print("SNMT")
ants.plot(os.path.join(img_path, snmt_files_wm[0]),axis=1)
print("NSMT")
ants.plot(os.path.join(img_path, nsmt_files_wm[0]),axis=1)
```

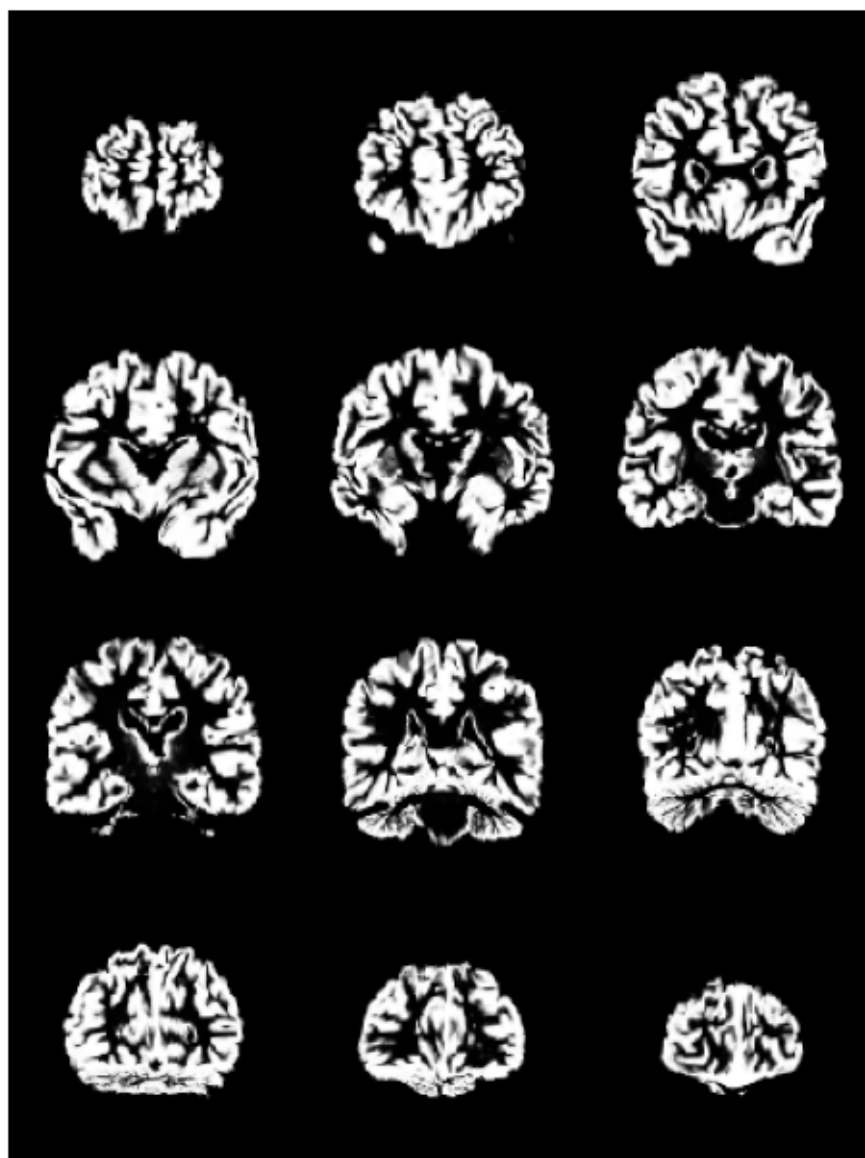
SMT



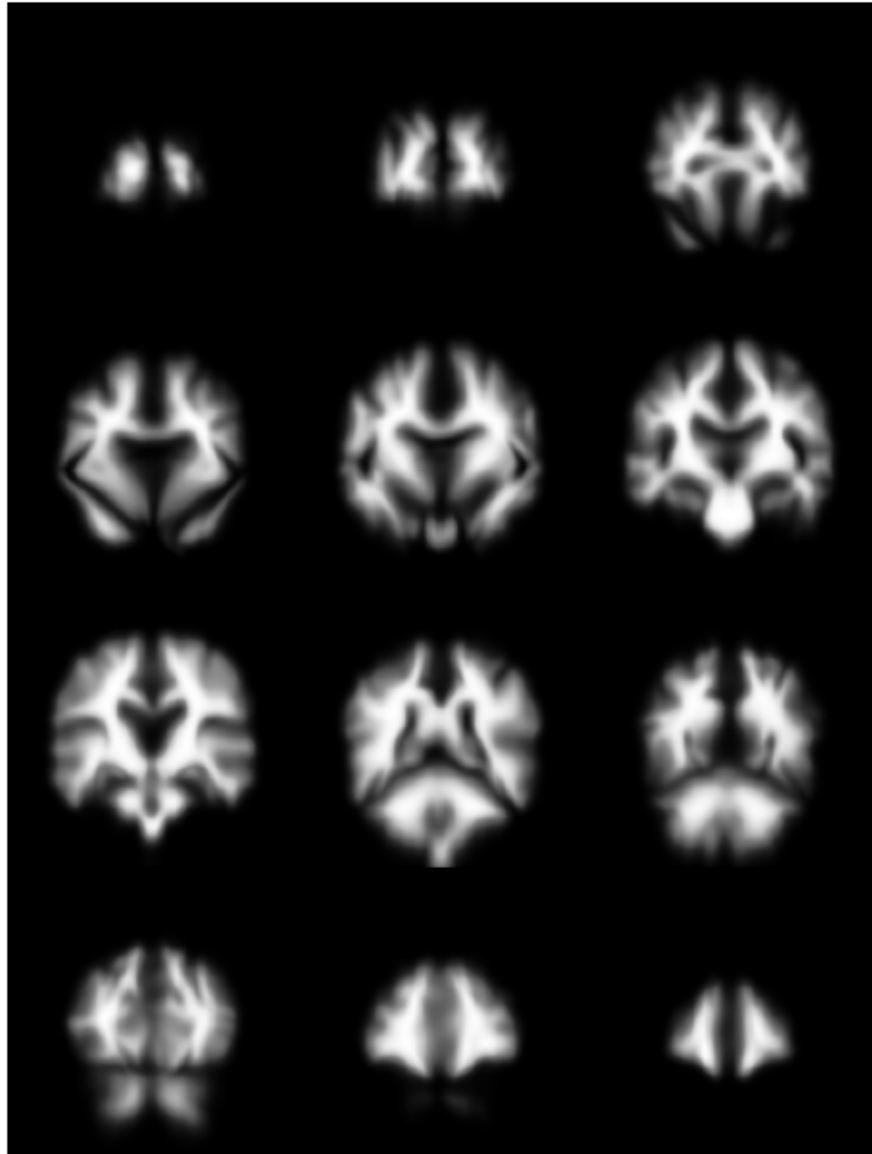
SNMT



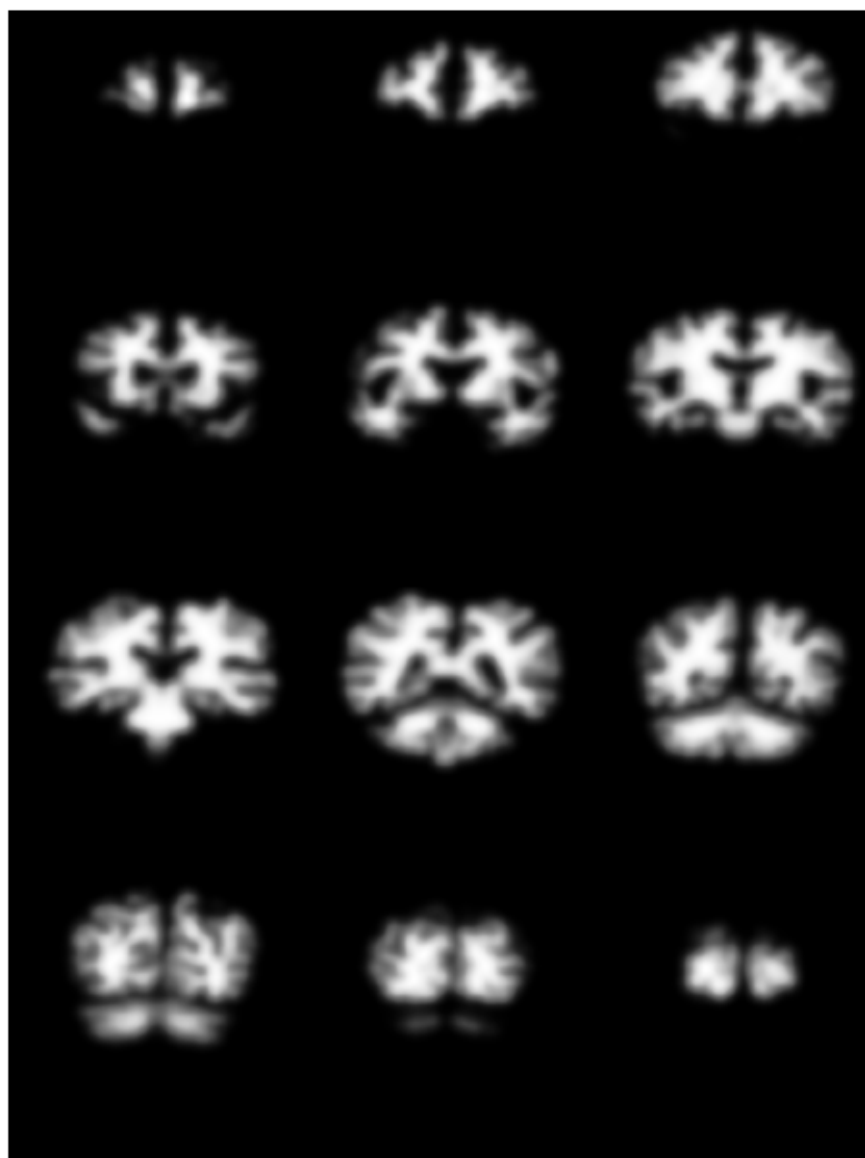
NSMT



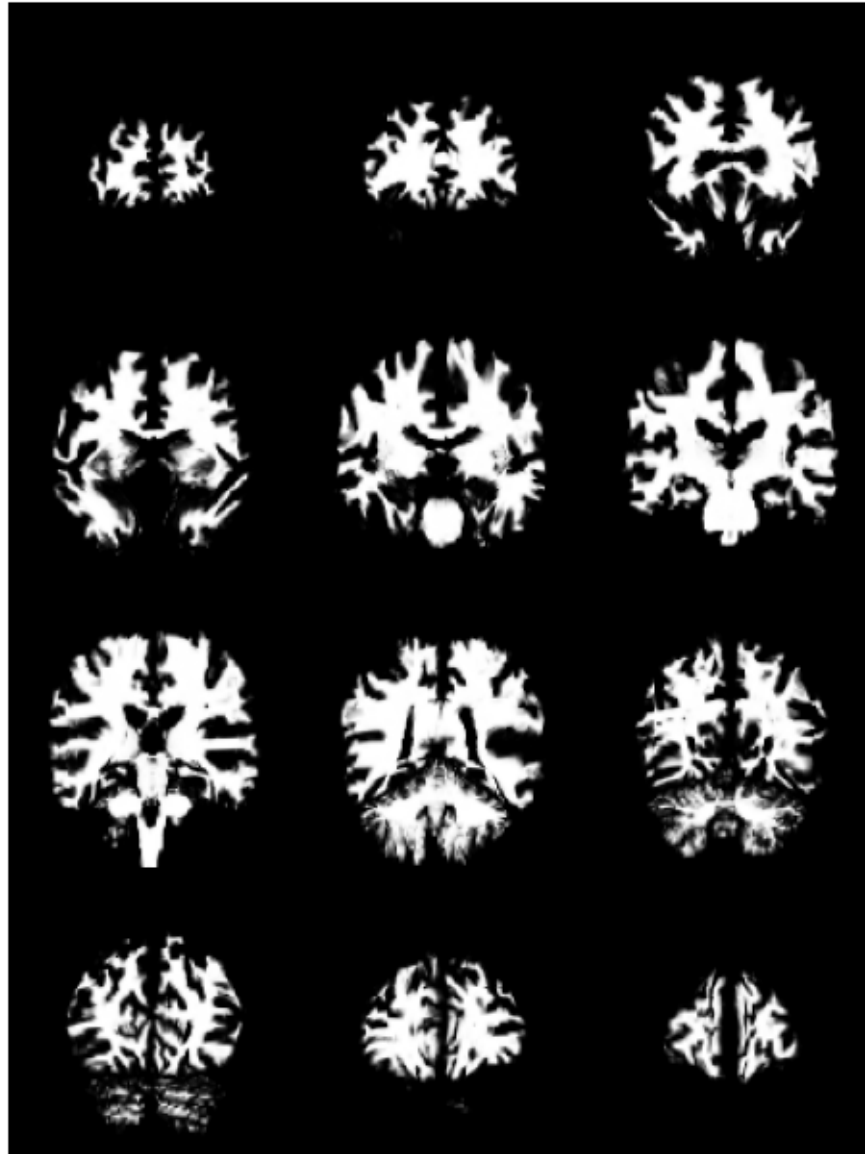
SMT



SNMT



NSMT



0.2 Create Design Matrix

```
[6]: def imgs_to_matrix(directory, wm_files=None, gm_files=None, combine=False):
      imgs = []

      if combine:

          for file_grouping in zip(wm_files, gm_files):
              wm_path, gm_path = file_grouping

              wm_img = ants.image_read(os.path.join(directory, wm_path))
```



```

gm_img = ants.image_read(os.path.join(directory, gm_path))

# Clone the white matter image
comb_img = ants.image_clone(wm_img)

# Add the gray matter image to the combined image
comb_img = comb_img + gm_img

# grab subject and img info
sub_id_wm, img_id_wm = wm_path.split('-')[1:3]
sub_id_gm, img_id_gm = gm_path.split('-')[1:3]

if sub_id_wm != sub_id_gm:
    raise ValueError(f'wm id:{sub_id_wm} ne to gm id:{sub_id_gm}')

vector = comb_img.numpy().ravel()

# turn to matrix, then to 1D array
img_vec = np.append([sub_id_wm, img_id_wm], vector)
imgs.append(img_vec)

X = np.vstack(imgs)
return X

else:
    all_files = [wm_files, gm_files]
    both_Xs = []
    for files in all_files:
        imgs = []
        for path in files:
            img = ants.image_read(os.path.join(directory, path))

            # grab subject and img info
            sub_id, img_id = path.split('-')[1:3]

            vector = img.numpy().ravel()

            # turn to matrix, then to 1D array
            img_vec = np.append([sub_id, img_id], vector)
            imgs.append(img_vec)

        # stack the vectors into a 2D array
        X = np.vstack(imgs)
        both_Xs.append(X)

# wm_X, gm_X
return both_Xs

```

```
[7]: def matrix_to_df(X):
    # V: Voxel intensity
    # turn matrix to dataframe and name columns
    X_cols = ['Subject', 'Img_ID'] + ['V{}'.format(i+1) for i in range(X.
↪shape[1]-2)]
    X_df = pd.DataFrame(X, columns=X_cols)

    return X_df

def clean_data(X_df, md):
    # merge two dfs
    X_cl = md.merge(X_df, on=['Subject', 'Img_ID'])
    X_cl = X_cl.drop(columns=['Img_ID', 'Subject'])

    # create X and y
    y = X_cl['Group'].values
    X = X_cl.drop(columns=['Group'])

    return X, y

def get_metadata(data_path):
    # Clean metadata dataframe
    md = pd.read_csv(os.path.join(data_path, 'ADNI1_Complete_2Yr_3T_4_18_2023.
↪csv'))

    md = md.rename(columns={'Image Data ID': 'Img_ID'})

    md = md.drop(columns=['Visit', 'Modality', 'Description', 'Type', 'Acq_
↪Date', 'Format', 'Downloaded'])

    md['Group'] = md['Group'].map({'CN':0, 'MCI':1, 'AD':2})
    md['Sex'] = md['Sex'].map({'F':0, 'M':1})

    return md
```

Testing out individual functions

```
[8]: X_wm, X_gm = imgs_to_matrix(img_path, smt_files_gm[0:5], smt_files_wm[0:5],
↪combine=False)
X_comb = imgs_to_matrix(img_path, smt_files_gm[0:5], smt_files_wm[0:5],
↪combine=True)
```

```
[9]: md = get_metadata(data_path)
md.head()
```

```
[9]:      Img_ID      Subject  Group  Sex  Age
0  I205567  136_S_1227      1    0   66
1   I66824  136_S_1227      1    0   65
2   I79080  136_S_1227      1    0   65
3  I143856  136_S_1227      1    0   67
4   I99265  136_S_1227      1    0   66
```

```
[10]: df = matrix_to_df(X_comb)
df.head()
```

```
[10]:      Subject  Img_ID  V1  V2  V3  V4  V5  V6  V7  V8  ... V2122936
0  002_S_0413  I118675  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0 \
1  002_S_0413  I120746  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0
2  002_S_0413  I128346  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0
3  002_S_0413  I40657   0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0
4  002_S_0413  I64551   0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0
```

```
      V2122937 V2122938 V2122939 V2122940 V2122941 V2122942 V2122943 V2122944
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
2      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
4      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
```

```
      V2122945
0      0.0
1      0.0
2      0.0
3      0.0
4      0.0
```

```
[5 rows x 2122947 columns]
```

```
[11]: X, y = df.pipe(clean_data, md=md)
```

```
[12]: X.head()
```

```
[12]:      Sex  Age  V1  V2  V3  V4  V5  V6  V7  V8  ... V2122936 V2122937
0     0   79  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0      0.0 \
1     0   76  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0      0.0
2     0   77  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0      0.0
3     0   76  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0      0.0
4     0   77  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  ...      0.0      0.0
```

```
      V2122938 V2122939 V2122940 V2122941 V2122942 V2122943 V2122944 V2122945
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
```

2	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
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

[5 rows x 2122947 columns]

0.3 PCA and Logistic Regression

```
[13]: def perform_pca(X, y):
    # Split the data into train and test sets
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
    random_state=10)

    # Preprocess and scale the data
    scaler = StandardScaler()
    X_train_scaled = scaler.fit_transform(X_train)
    X_test_scaled = scaler.transform(X_test)

    # Fit and transform the PCA model on the training set
    pca = PCA(random_state=10)

    X_train_pca = pca.fit_transform(X_train_scaled)

    # calculate cumulative variance
    cumulative_variance = np.cumsum(pca.explained_variance_ratio_)

    # find the index where cumulative variance reaches 95%
    n_components = np.argmax(cumulative_variance >= 0.95) + 1
    print(f'n components:{n_components}')

    # re-fit PCA with the chosen number of components
    pca = PCA(n_components=n_components, random_state=10)
    X_train_pca = pca.fit_transform(X_train_scaled)

    # Transform the test set using the trained PCA model
    X_test_pca = pca.transform(X_test_scaled)

    return X_train_pca, y_train, X_test_pca, y_test

def perform_logreg(X_train_pca, y_train, X_test_pca, y_test):
    clf = LogisticRegression(random_state=10, penalty=None,
    multi_class='multinomial', max_iter=1000).fit(X_train_pca, y_train)
    y_preds = clf.predict(X_test_pca)

    acc = sum(y_preds == y_test) / len(y_test)
```

```

    return acc

def full_pipeline(X_matrix):

    md = get_metadata(data_path)

    df = matrix_to_df(X_matrix)

    X, y = df.pipe(clean_data, md=md)

    X_train_pca, y_train, X_test_pca, y_test = perform_pca(X, y)

    return X_train_pca, y_train, X_test_pca, y_test

```

0.4 Comparisons

```

[14]: X_wm, X_gm = imgs_to_matrix(img_path, smt_files_gm, smt_files_wm, combine=False)
      X_comb = imgs_to_matrix(img_path, smt_files_gm, smt_files_wm, combine=True)

```

```

[15]: X_train_wm, y_train_wm, X_test_wm, y_test_wm = full_pipeline(X_wm)
      X_train_gm, y_train_gm, X_test_gm, y_test_gm = full_pipeline(X_gm)
      X_train_cb, y_train_cb, X_test_cb, y_test_cb = full_pipeline(X_comb)

```

```

n components:147
n components:160
n components:175

```

```

[16]: base_pca_dir = os.path.join(data_path, 'base_pca_data')
      os.makedirs(base_pca_dir, exist_ok=True)

      arrs = {'X_train_wm': X_train_wm, 'y_train_wm': y_train_wm,
              'X_test_wm': X_test_wm, 'y_test_wm': y_test_wm,
              'X_train_gm': X_train_gm, 'y_train_gm': y_train_gm,
              'X_test_gm': X_test_gm, 'y_test_gm': y_test_gm,
              'X_train_cb': X_train_cb, 'y_train_cb': y_train_cb,
              'X_test_cb': X_test_cb, 'y_test_cb': y_test_cb,
              }

      # loop through the dictionary and save each dataframe to CSV file
      for name, arr in arrs.items():
          np.savetxt(os.path.join(base_pca_dir, f'{name}.csv'), arr, delimiter=',')

```

```

[17]: logreg_wm_acc = perform_logreg(X_train_wm, y_train_wm, X_test_wm, y_test_wm)
      logreg_gm_acc = perform_logreg(X_train_gm, y_train_gm, X_test_gm, y_test_gm)
      logreg_cb_acc = perform_logreg(X_train_cb, y_train_cb, X_test_cb, y_test_cb)

```

```
[18]: print(f"Classification accuracy under WM data: {logreg_wm_acc}")
      print(f"Classification accuracy under GM data: {logreg_gm_acc}")
      print(f"Classification accuracy under Combined data: {logreg_cb_acc}")
```

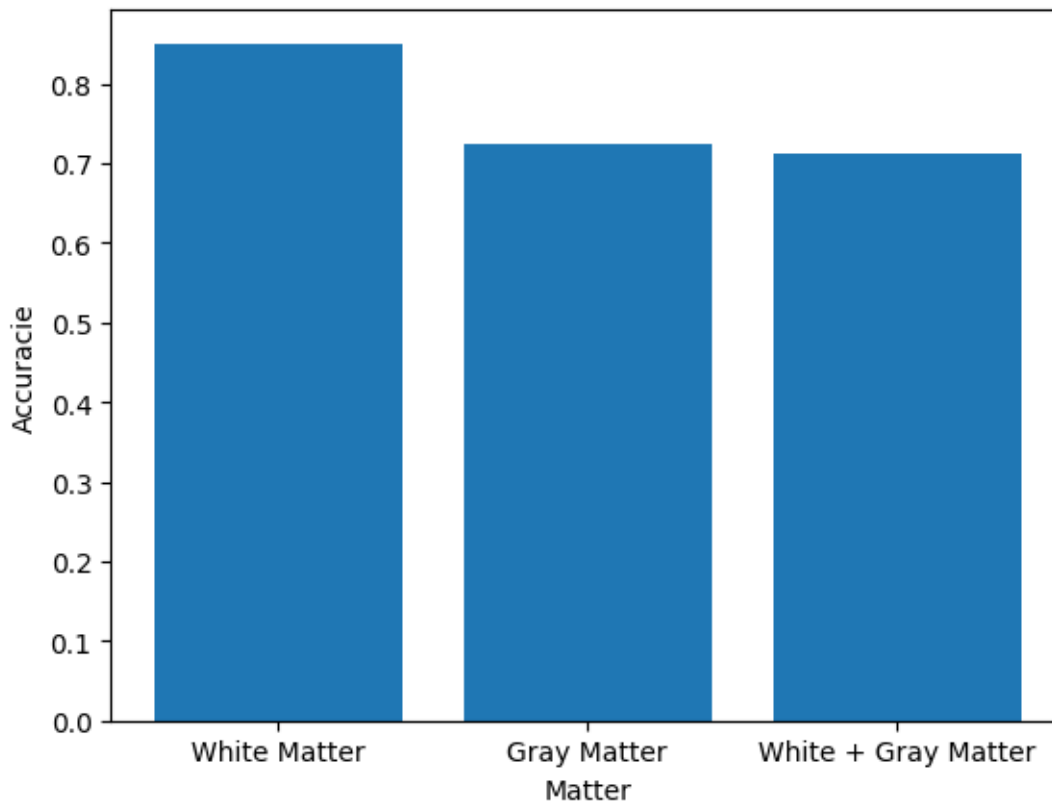
Classification accuracy under WM data: 0.8505747126436781

Classification accuracy under GM data: 0.7241379310344828

Classification accuracy under Combined data: 0.7126436781609196

```
[19]: # Create a bar plot
      accuracies = [logreg_wm_acc, logreg_gm_acc, logreg_cb_acc]
      labels = ['White Matter', 'Gray Matter', 'White + Gray Matter']
      plt.bar(labels, accuracies)

      # Add labels and title
      plt.xlabel('Matter')
      plt.ylabel('Accuracie')
      # plt.title('Bar plot of 3 values')
      # Show the plot
      plt.show()
```



Using white matter data for cross validation

```
[20]: from sklearn.model_selection import GridSearchCV

# define logistic regression model
lr = LogisticRegression(multi_class='multinomial', random_state=10,
    ↪penalty=None, max_iter=1000)

# define solvers to test
solvers = ['lbfgs', 'newton-cg', 'sag', 'saga']

# define grid search parameters
param_grid = {'solver': solvers}

# perform grid search
grid_search = GridSearchCV(lr, param_grid=param_grid, cv=5)
grid_search.fit(X_train_wm, y_train_wm)

# get the best model
best_model = grid_search.best_estimator_
print(best_model)

# use the best model to make predictions on the test set
y_preds = best_model.predict(X_test_wm)

acc = sum(y_preds == y_test_wm) / len(y_test_wm)
print(f"{best_model} has accuracy: {acc}")
```

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

The max_iter was reached which means the coef_ did not converge

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

The max_iter was reached which means the coef_ did not converge

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

The max_iter was reached which means the coef_ did not converge

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

The max_iter was reached which means the coef_ did not converge

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-
```

```
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

```
The max_iter was reached which means the coef_ did not converge
```

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-  
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

```
The max_iter was reached which means the coef_ did not converge
```

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-  
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

```
The max_iter was reached which means the coef_ did not converge
```

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-  
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

```
The max_iter was reached which means the coef_ did not converge
```

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-  
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

```
The max_iter was reached which means the coef_ did not converge
```

```
/scratch/users/neuroimage/conda/venv/lib/python3.11/site-  
packages/sklearn/linear_model/_sag.py:350: ConvergenceWarning:
```

```
The max_iter was reached which means the coef_ did not converge
```

```
LogisticRegression(max_iter=1000, multi_class='multinomial', penalty=None,  
                    random_state=10)
```

```
LogisticRegression(max_iter=1000, multi_class='multinomial', penalty=None,  
                    random_state=10) has accuracy: 0.8505747126436781
```

```
[ ]:
```