ABIDE_PCA_analysis

March 24, 2023

[1]:
```
import numpy as np
import pandas as pd
from dask import dataframe as dd
import matplotlib.pyplot as plt
from scipy.stats import kendalltau, rankdata, norm
# import fastHDMI as mi
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler, SplineTransformer
from sklearn.decomposition import PCA
from sklearn.linear_model import LassoCV, ElasticNetCV, RidgeCV, LarsCV,␣
 ↪LassoLarsCV, LogisticRegressionCV, LinearRegression, LogisticRegression
from sklearn.neural_network import MLPRegressor, MLPClassifier
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score, roc_auc_score
import multiprocess as mp
from tqdm import tqdm
import os
```

1 Calculate MI for ABIDE data age and diagnosis outcome

1.1 this block is only to be run on Compute Canada

[2]:
```
# # running PCA on it

# import numpy as np
# import pandas as pd
# from dask import dataframe as dd
# import matplotlib.pyplot as plt
# from scipy.stats import kendalltau, rankdata, norm
# import fastHDMI as mi
# from sklearn.model_selection import train_test_split, GridSearchCV
# from sklearn.preprocessing import StandardScaler, SplineTransformer
# from sklearn.decomposition import PCA
# from sklearn.linear_model import LassoCV, ElasticNetCV, RidgeCV, LarsCV,␣
 ↪LassoLarsCV, LogisticRegressionCV, LinearRegression, LogisticRegression
# from sklearn.neural_network import MLPRegressor, MLPClassifier
# from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
```

```
# from sklearn.metrics import r2_score, roc_auc_score
# import multiprocess as mp
# from tqdm import tqdm
# import os

# csv_file = os.environ["SLURM_TMPDIR"] + \
#     r"/ABIDE_PCA.csv"
# abide = pd.read_csv(csv_file, encoding="unicode_escape", engine="c")
# _sex = abide["SEX"].tolist()
# _age = abide["AGE_AT_SCAN"].tolist()
# _diagnosis = abide["DX_GROUP"].tolist()
# abide = abide.iloc[:, 2:-3].to_numpy(copy=False)
# abide = StandardScaler(copy=False).fit_transform(abide)

# pca = PCA(n_components=abide.shape[0])
# components = pca.fit(
#     abide
# ).components_.T  # transpose because it's a ndarray of shape (n_components,
 ↪n_features)
# pca_output = abide @ components
# cols = ["PC_" + str(j + 1) for j in range(pca_output.shape[1])]
# df = pd.DataFrame(pca_output, columns=cols)
# df["SEX"] = _sex
# df["AGE_AT_SCAN"] = _age
# df["DX_GROUP"] = _diagnosis
# df.to_csv(r"./ABIDE_PCA/ABIDE_PCA.csv")
```

[3]:
```
from pathlib import Path


def engine_and_share_memory_status(mem_setting):
    if mem_setting == "high_mem":
        return "c", False
    elif mem_setting == "share_mem":
        return "c", True
    elif mem_setting == "dask":
        return "dask", False


def job_generator(mem_setting, outcome):
    py_1 = r"""import numpy as np
import pandas as pd
from dask import dataframe as dd
import matplotlib.pyplot as plt
from scipy.stats import kendalltau, rankdata, norm
import fastHDMI as mi
from sklearn.model_selection import train_test_split, GridSearchCV
```

```
from sklearn.preprocessing import StandardScaler, SplineTransformer
from sklearn.decomposition import PCA
from sklearn.linear_model import LassoCV, ElasticNetCV, RidgeCV, LarsCV,␣
 ↪LassoLarsCV, LogisticRegressionCV, LinearRegression, LogisticRegression
from sklearn.neural_network import MLPRegressor, MLPClassifier
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score, roc_auc_score
import multiprocess as mp
from tqdm import tqdm
import os

csv_file = os.environ["SLURM_TMPDIR"] + \
    r"/ABIDE_PCA.csv"
# abide = pd.read_csv(csv_file, encoding="unicode_escape", engine="c")
abide = dd.read_csv(csv_file, sample=1250000)

# _abide_name = abide.columns.tolist()[1:]
_abide_name = list(abide.columns)[1:]

# print(_abide_name)

# we don't inlcude age and sex in the screening since we choose to always␣
 ↪include them in the model
"""
    if outcome == "age":
        py_2 = r"""
abide_name = [_abide_name[-2]] + _abide_name[:-3]
# so that the left first column is the outcome and the rest columns are areas

np.save(r"./ABIDE_columns", _abide_name[:-3])

del _abide_name

print("The outcome is age.")
print(
    "Now running using {_csv_engine} CSV engine with␣
 ↪share_memory={_share_mem_status}."
)
print("Our developed FFT-based MI calculation:")

for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        try:
            mi_output = mi.continuous_screening_csv_parallel(
```

```
                csv_file,
                _usecols=abide_name.copy(),
                csv_engine="{_csv_engine}",
                sample=1250000,
                multp=10,
                core_num=10,
                share_memory={_share_mem_status},
                kernel=_kernel,
                bw=_bw,
                norm=2)
            if "{mem_setting}" == "high_mem":
                np.save(
                    r"./ABIDE_age_MI_{{kernel}}_{{bw}}_output".format(
                        kernel=_kernel, bw=_bw), mi_output)

            del mi_output

        except:
            print("This kernel-bw combination reports an error: ", _kernel,
                  _bw)

print("sklearn MI calculation:")

skmi_output = mi.continuous_skMI_screening_csv_parallel(
    csv_file,
    _usecols=abide_name.copy(),
    csv_engine="{_csv_engine}",
    sample=1250000,
    multp=10,
    core_num=10,
    random_state=0,
    share_memory={_share_mem_status})
if "{mem_setting}" == "high_mem":
    np.save(r"./ABIDE_age_skMI_output", skmi_output)

del skmi_output

print("Pearson's correlation calculation:")

pearson_output = mi.Pearson_screening_csv_parallel(
    csv_file,
    _usecols=abide_name.copy(),
    csv_engine="{_csv_engine}",
    sample=1250000,
    multp=10,
    core_num=10,
    share_memory={_share_mem_status})
```

```
if "{mem_setting}" == "high_mem":
    np.save(r"./ABIDE_age_Pearson_output", pearson_output)

del pearson_output
""".format(_csv_engine=engine_and_share_memory_status(mem_setting)[0],
           _share_mem_status=engine_and_share_memory_status(mem_setting)[1],
           mem_setting=mem_setting)
    elif outcome == "diagnosis":
        py_2 = r"""
abide_name = [_abide_name[-1]] + _abide_name[:-3]
# so that the left first column is the outcome and the rest columns are areas

del _abide_name

print("The outcome is diagnosis.")
print(
    "Now running using {_csv_engine} CSV engine with␣
 ↪share_memory={_share_mem_status}."
)
print("Our developed FFT-based MI calculation:")

for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        try:
            mi_output = mi.binary_screening_csv_parallel(
                csv_file,
                _usecols=abide_name.copy(),
                csv_engine="{_csv_engine}",
                sample=1250000,
                multp=10,
                core_num=10,
                share_memory={_share_mem_status},
                kernel=_kernel,
                bw=_bw)
            if "{mem_setting}" == "high_mem":
                np.save(
                    r"./ABIDE_diagnosis_MI_{{kernel}}_{{bw}}_output".format(
                        kernel=_kernel, bw=_bw), mi_output)

            del mi_output

        except:
            print("This kernel-bw combination reports an error: ", _kernel,
                  _bw)
```

```
print("sklearn MI calculation:")

skmi_output = mi.binary_skMI_screening_csv_parallel(
    csv_file,
    _usecols=abide_name.copy(),
    csv_engine="{_csv_engine}",
    sample=1250000,
    multp=10,
    core_num=10,
    random_state=0,
    share_memory={_share_mem_status})
if "{mem_setting}" == "high_mem":
    np.save(r"./ABIDE_diagnosis_skMI_output", skmi_output)

del skmi_output

print("Pearson's correlation calculation:")

pearson_output = mi.Pearson_screening_csv_parallel(
    csv_file,
    _usecols=abide_name.copy(),
    csv_engine="{_csv_engine}",
    sample=1250000,
    multp=10,
    core_num=10,
    share_memory={_share_mem_status})
if "{mem_setting}" == "high_mem":
    np.save(r"./ABIDE_diagnosis_Pearson_output", pearson_output)

del pearson_output
""".format(_csv_engine=engine_and_share_memory_status(mem_setting)[0],
           _share_mem_status=engine_and_share_memory_status(mem_setting)[1],
           mem_setting=mem_setting)

    Path(r"./ABIDE_screening_" + outcome + "_" + mem_setting + ".py").touch()
    py_script = open(
        r"./ABIDE_screening_" + outcome + "_" + mem_setting + ".py", "w")
    py_script.write(py_1 + py_2)

    Path(r"./ABIDE_screening_" + outcome + "_" + mem_setting + ".sh").touch()
    bash_script = open(
        r"./ABIDE_screening_" + outcome + "_" + mem_setting + ".sh", "w")
    bash_script.write(r"""#!/bin/bash
#SBATCH --account=def-masd
#SBATCH --nodes=1
#SBATCH --cpus-per-task=10
```

```
#SBATCH --mem=80G
#SBATCH --time=20:00:00
#SBATCH --job-name=ABIDE_screening_{outcome}_{mem_setting}

module load gcc llvm rust arrow cuda nodejs python/3.8.10 r/4.0.2␣
 ↪python-build-bundle

virtualenv --no-download $SLURM_TMPDIR/env
source $SLURM_TMPDIR/env/bin/activate
pip install --no-index --upgrade pip

# ### run this block at the login node to build wheels
# ### get wheels builder
# git clone https://github.com/ComputeCanada/wheels_builder
# export PATH=$PATH:${{HOME}}/wheels_builder
# ### build KDEpy 1.1.0
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package KDEpy --version 1.1.0␣
 ↪--python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/packages/
# ### built nonconvexAG 1.0.6
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package nonconvexAG --version 1.
 ↪0.6 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/
# ### built fastHDMI 1.18.20
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package fastHDMI --version 1.18.
 ↪20 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/

# Here basically to build the packages at login node and install them in slurm␣
 ↪job submission locally
pip install --no-index bed-reader numpy sklearn matplotlib scipy numba␣
 ↪multiprocess scikit-learn cupy rpy2
pip install --no-index /home/kyang/KDEpy-1.1.
 ↪0+computecanada-cp38-cp38-linux_x86_64.whl
pip install --no-index /home/kyang/nonconvexAG-1.0.6+computecanada-py3-none-any.
 ↪whl
pip install --no-index /home/kyang/fastHDMI-1.18.20+computecanada-py3-none-any.
 ↪whl

nvidia-smi
lscpu

echo "running ABIDE_screening_{outcome}_{mem_setting}.py"

cp /home/kyang/ABIDE_data_analysis/ABIDE_PCA/ABIDE_PCA.csv $SLURM_TMPDIR/

python3 ABIDE_screening_{outcome}_{mem_setting}.py
```

```
""".format(outcome=outcome, mem_setting=mem_setting))


for mem_setting in ["high_mem", "share_mem", "dask"]:
    for outcome in ["age", "diagnosis"]:
        job_generator(mem_setting=mem_setting, outcome=outcome)
```

[4]:
```
#!find . -name "*.py" -exec yapf --in-place "{}" \;
#!find . -name "*.py" -exec autopep8 --in-place "{}" \;
# !find . -name "*.py" -exec yapf --in-place "{}" \;
# !find . -name "*.py" -exec autopep8 --in-place "{}" \;
```

2 Plots for age

2.1 Comparing two ranking with Kendall'sτ

The results show that the two ranking by mutual information and Pearson's correlation vary greatly by Kendall'stau – I also tried the Pearson's correlation between two ranking (not that I should do this) and the correlation is also very small.

So in summary, the two ranking vary somehow.

[5]:
```
# abide_mi = np.load(r"./ABIDE_age_MI_output.npy")
# plt.hist(np.log(abide_mi), 500)
# plt.show()

# abide_pearson = np.load(r"./ABIDE_age_Pearson_output.npy")
# plt.hist(np.log(np.abs(abide_pearson)), 500)
# plt.show()

# abide_skmi = np.load(r"./ABIDE_age_skMI_output.npy")
# plt.hist(np.log(np.abs(abide_pearson)), 500)
# plt.show()

# print("Kendall'stau for MI vs Pearson: \n",
#       kendalltau(rankdata(-abide_mi), rankdata(-np.abs(abide_pearson))))

# plt.scatter(np.log(abide_mi), abide_pearson, s=10,
#             alpha=.2)  # s is the dot size
# plt.show()
# # keep this, add different selections
# # PREDICT AGE

# print("Kendall'stau for MI vs skMI: \n",
#       kendalltau(rankdata(-abide_mi), rankdata(-np.abs(abide_skmi))))

# plt.scatter(np.log(abide_mi), abide_skmi, s=10, alpha=.2)  # s is the dot size
# plt.show()
```

```
# # keep this, add different selections
# # PREDICT AGE
```

3 Plots for diagnosis

[6]:
```
# abide_mi = np.load(r"./ABIDE_diagnosis_MI_output.npy")
# plt.hist(np.log(abide_mi), 500)
# plt.show()

# abide_pearson = np.load(r"./ABIDE_diagnosis_Pearson_output.npy")
# plt.hist(np.log(np.abs(abide_pearson)), 500)
# plt.show()

# abide_skmi = np.load(r"./ABIDE_diagnosis_skMI_output.npy")
# plt.hist(np.log(np.abs(abide_pearson)), 500)
# plt.show()

# print("Kendall'stau for MI vs Pearson: \n",
#       kendalltau(rankdata(-abide_mi), rankdata(-np.abs(abide_pearson))))

# plt.scatter(np.log(abide_mi), abide_pearson, s=10,
#             alpha=.2)  # s is the dot size
# plt.show()
# # keep this, add different selections
# # PREDICT diagnosis

# print("Kendall'stau for MI vs skMI: \n",
#       kendalltau(rankdata(-abide_mi), rankdata(-np.abs(abide_skmi))))

# plt.scatter(np.log(abide_mi), abide_skmi, s=10, alpha=.2)  # s is the dot size
# plt.show()
# # keep this, add different selections
# # PREDICT diagnosis
```

4 Try Fitting models to predict age, 5-fold CV

4.1 this block of code only means to be run on Compute Canada

4.1.1 ABIDE_predict_age

[7]:
```
from pathlib import Path


def job_creator(dep_measure, fun_name):
    Path(r"./ABIDE_predict_age/ABIDE_age_" + dep_measure + "_" + fun_name +
         ".sh").touch()
```

```
    Path(r"./ABIDE_predict_age/ABIDE_age_" + dep_measure + "_" + fun_name +
         ".py").touch()
    bash_script = open(
        r"./ABIDE_predict_age/ABIDE_age_" + dep_measure + "_" + fun_name +
        ".sh", "w")
    py_script = open(
        r"./ABIDE_predict_age/ABIDE_age_" + dep_measure + "_" + fun_name +
        ".py", "w")
    bash_script.write(r"""#!/bin/bash
#SBATCH --account=def-masd
#SBATCH --nodes=1
#SBATCH --cpus-per-task=10
#SBATCH --mem=80G
#SBATCH --time=3-12:00:00
#SBATCH --job-name=age_{dep_measure}_{fun_name}

module load gcc llvm rust arrow cuda nodejs python/3.8.10 r/4.0.2␣
 ↪python-build-bundle

virtualenv --no-download $SLURM_TMPDIR/env
source $SLURM_TMPDIR/env/bin/activate
pip install --no-index --upgrade pip

# ### run this block at the login node to build wheels
# ### get wheels builder
# git clone https://github.com/ComputeCanada/wheels_builder
# export PATH=$PATH:${{HOME}}/wheels_builder
# ### build KDEpy 1.1.0
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package KDEpy --version 1.1.0␣
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# ### built nonconvexAG 1.0.6
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 ↪packages/
# ### built fastHDMI 1.18.20
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package fastHDMI --version 1.18.
 ↪20 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/

# Here basically to build the packages at login node and install them in slurm␣
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pip install --no-index bed-reader numpy sklearn matplotlib scipy numba␣
 ↪multiprocess scikit-learn cupy rpy2
pip install --no-index /home/kyang/KDEpy-1.1.
 ↪0+computecanada-cp38-cp38-linux_x86_64.whl
```

```
pip install --no-index /home/kyang/nonconvexAG-1.0.6+computecanada-py3-none-any.
 ↪whl
pip install --no-index /home/kyang/fastHDMI-1.18.20+computecanada-py3-none-any.
 ↪whl

nvidia-smi
lscpu

echo "running ABIDE_age_{dep_measure}_{fun_name}.py"

cp /home/kyang/ABIDE_data_analysis/ABIDE_PCA/ABIDE_PCA.csv $SLURM_TMPDIR/
cp ../ABIDE_columns.npy $SLURM_TMPDIR/
cp ../ABIDE_age_{dep_measure}_output.npy $SLURM_TMPDIR/

python3 ABIDE_age_{dep_measure}_{fun_name}.py
    """.format(dep_measure=dep_measure, fun_name=fun_name))
    py_script.write(r"""import numpy as np
import pandas as pd
from dask import dataframe as dd
import matplotlib.pyplot as plt
from scipy.stats import kendalltau, rankdata, norm
import fastHDMI as mi
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler, SplineTransformer
from sklearn.decomposition import PCA
from sklearn.linear_model import LassoCV, ElasticNetCV, RidgeCV, LarsCV,␣
 ↪LassoLarsCV, LogisticRegressionCV, LinearRegression, LogisticRegression
from sklearn.neural_network import MLPRegressor, MLPClassifier
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score, roc_auc_score
import multiprocess as mp
from tqdm import tqdm
import os

csv_file = os.environ["SLURM_TMPDIR"] + \
    r"/ABIDE_PCA.csv"
original_df = pd.read_csv(csv_file, encoding="unicode_escape", engine="c")

columns = np.load(os.environ["SLURM_TMPDIR"] + r"/ABIDE_columns.npy")
abide_dep = np.load(os.environ["SLURM_TMPDIR"] +
                    r"/ABIDE_age_{dep_measure}_output.npy")  # dep_measure
abide_dep = np.absolute(abide_dep)


def binning(var, num_bins, min_num=2):
    bins = np.linspace(np.min(var) - 1e-8, np.max(var) + 1e-8, num_bins)
    var_binned = np.digitize(var, bins)
```

```
    category = np.sort(np.unique(var_binned))
    while len([
            x for x in category if np.count_nonzero(var_binned == x) < min_num
    ]) != 0:
        for j in range(len(category)):
            if j < len(
                    category
            ):  # since category is always updated, we add this to avoid out of␣
 ↪index error; alternatively, a while loop also works
                if np.count_nonzero(
                        var_binned == category[j]
                ) < min_num:  # if the number of observations in a category is␣
 ↪less than min_num
                    if j == 0:  # if it's the first category, combine it with␣
 ↪the second
                        var_binned[var_binned == category[j]] = category[j + 1]
                    else:  # if it's not the first category, combine it with␣
 ↪the previous one
                        var_binned[var_binned == category[j]] = category[j - 1]
                    category = np.sort(np.unique(var_binned))
    return var_binned


def LogisticRegressionCV_l1(**arg):
    return LogisticRegressionCV(penalty="l1",
                                solver="saga",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_l2(**arg):
    return LogisticRegressionCV(penalty="l2",
                                solver="lbfgs",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_ElasticNet(**arg):
    return LogisticRegressionCV(penalty="elasticnet",
                                solver="saga",
                                multi_class="ovr",
                                l1_ratios=np.linspace(0, 1, 12)[1:-1],
                                **arg)


def testing_error(num_covariates=20,
                  training_proportion=.8,
```

```
                fun=ElasticNetCV,
                outcome_name="AGE_AT_SCAN",
                seed=1):
    np.random.seed(seed)
    _usecols = np.hstack((
        outcome_name,  # "SEX", "DX_GROUP",
        columns[np.argsort(-abide_dep)][:num_covariates]))
    df = original_df[_usecols].dropna(inplace=False).sample(
        frac=1, random_state=seed, replace=False).reset_index(drop=True,
                                                              inplace=False)
    if df.shape[0] > 20:
        X, y = df.iloc[:,
                       1:].to_numpy(copy=True), df.iloc[:,
                                                        0].to_numpy(copy=True)
        X = StandardScaler(copy=False).fit_transform(X)
        # if the outcome is continuous, we have to use binning
        if fun in [
                ElasticNetCV, LassoCV, RidgeCV, LarsCV, LassoLarsCV,
                MLPRegressor, RandomForestRegressor, LinearRegression
        ]:
            y_binned = binning(y, 30, min_num=2)
        else:
            y_binned = y.copy()
        X_train, X_test, y_train, y_test = train_test_split(
            X,
            y,
            train_size=training_proportion,
            random_state=seed,
            stratify=y_binned)
        if fun in [ElasticNetCV, LassoCV]:
            fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [RidgeCV]:  # RidgeCV doesn't have seed setting and n_jobs
            fit = fun(cv=5).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [LarsCV, LassoLarsCV
                     ]:  # LarsCV doesn't have seed setting but have n_jobs
            fit = fun(cv=5, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [MLPRegressor]:
            mlp_gs = fun(random_state=seed, max_iter=500)
            parameter_space = {{
                "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                       (500, )],
```

```
            "activation": ["tanh", "relu"],
            "solver": ["sgd", "adam"],
            "alpha": [0.0001, 0.05],
            "learning_rate": ["constant", "adaptive"]
        }}
        clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
        clf.fit(X_train, y_train)
        y_pred = clf.predict(X_test)
        out = r2_score(y_test, y_pred)
    elif fun in [MLPClassifier]:
        mlp_gs = fun(random_state=seed, max_iter=500)
        parameter_space = {{
            "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                   (500, )],
            "activation": ["tanh", "relu"],
            "solver": ["sgd", "adam"],
            "alpha": [0.0001, 0.05],
            "learning_rate": ["constant", "adaptive"]
        }}
        clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
        clf.fit(X_train, y_train)
        y_pred = clf.predict_proba(
            X_test)[:, 1]  # predict probability to calculate ROC
        out = roc_auc_score(y_test, y_pred)
    elif fun in [
            LogisticRegressionCV_l1, LogisticRegressionCV_l2,
            LogisticRegressionCV_ElasticNet
    ]:
        fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
        y_pred = fit.predict_proba(
            X_test)[:, 1]  # predict probability to calculate ROC
        out = roc_auc_score(y_test, y_pred)
    elif fun in [RandomForestRegressor]:
        fit = fun(random_state=seed, n_jobs=10,
                  n_estimators=500).fit(X_train, y_train)
        y_pred = fit.predict(X_test)
        out = r2_score(y_test, y_pred)
    elif fun in [RandomForestClassifier]:
        fit = fun(random_state=seed, n_jobs=10,
                  n_estimators=500).fit(X_train, y_train)
        y_pred = fit.predict_proba(
            X_test)[:, 1]  # predict probability to calculate ROC
        out = roc_auc_score(y_test, y_pred)
    elif fun in [LinearRegression]:
        fit = fun(n_jobs=10).fit(X_train, y_train)
        y_pred = fit.predict(X_test)
        out = r2_score(y_test, y_pred)
```

```
        elif fun in [LogisticRegression]:
            fit = fun(penalty=None, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
    else:
        out = np.nan
    return out


def testing_error_rep(num_covariates=20,
                      training_proportion=.8,
                      fun=ElasticNetCV,
                      outcome_name="AGE_AT_SCAN",
                      num_rep=10):
    def _testing_error(seed):
        return testing_error(num_covariates=num_covariates,
                             training_proportion=training_proportion,
                             fun=fun,
                             outcome_name=outcome_name,
                             seed=seed)

    seeds = np.arange(num_rep)
    return np.array(list(map(_testing_error, seeds)))


def testing_error_num_attr(num_attr,
                           training_proportion=.8,
                           fun=ElasticNetCV,
                           outcome_name="AGE_AT_SCAN",
                           num_rep=10):
    def _testing_error_rep(_num_attr):
        return testing_error_rep(num_covariates=_num_attr,
                                 training_proportion=training_proportion,
                                 fun=fun,
                                 outcome_name=outcome_name,
                                 num_rep=num_rep)

    return np.array(list(map(_testing_error_rep, tqdm(num_attr))))


print(r"ABIDE_age_{dep_measure}_{fun_name}")  # dep_measure, fun_name
output = testing_error_num_attr(
    num_attr=list(map(int,
                      np.around(np.linspace(0, 50, 10 + 1)[1:]).tolist())),
    training_proportion=.8,  # 80/20 training+validation/testing division
    fun={fun_name},  # fun_name
```

```
    outcome_name="AGE_AT_SCAN",
    num_rep=20)
np.save(r"./ABIDE_age_{dep_measure}_{fun_name}",
        output)  # dep_measure, fun_name
    """.format(dep_measure=dep_measure, fun_name=fun_name))


dep_measure_list = []
for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]

for fun_name in [
        "LassoCV", "ElasticNetCV", "RidgeCV", "LarsCV", "LassoLarsCV",
        "MLPRegressor", "RandomForestRegressor", "LinearRegression"
]:
    for dep_measure in [*dep_measure_list, "Pearson", "skMI"]:
        job_creator(dep_measure, fun_name)
```

[8]:
```
#!find . -name "*.py" -exec yapf --in-place "{}" \;
#!find . -name "*.py" -exec autopep8 --in-place "{}" \;
# !find . -name "*.py" -exec yapf --in-place "{}" \;
# !find . -name "*.py" -exec autopep8 --in-place "{}" \;
```

4.1.2 ABIDE_poly3_predict_age

[9]:
```
from pathlib import Path


def job_creator(dep_measure, fun_name):
    Path(r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_" + dep_measure + "_" +
         fun_name + ".sh").touch()
    Path(r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_" + dep_measure + "_" +
         fun_name + ".py").touch()
    bash_script = open(
        r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_" + dep_measure + "_" +
        fun_name + ".sh", "w")
    py_script = open(
        r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_" + dep_measure + "_" +
        fun_name + ".py", "w")
    bash_script.write(r"""#!/bin/bash
#SBATCH --account=def-cgreenwo
#SBATCH --nodes=1
#SBATCH --cpus-per-task=10
```

```
#SBATCH --mem=80G
#SBATCH --time=3-12:00:00
#SBATCH --job-name=poly3_age_{dep_measure}_{fun_name}

module load gcc llvm rust arrow cuda nodejs python/3.8.10 r/4.0.2␣
 ↪python-build-bundle

virtualenv --no-download $SLURM_TMPDIR/env
source $SLURM_TMPDIR/env/bin/activate
pip install --no-index --upgrade pip

# ### run this block at the login node to build wheels
# ### get wheels builder
# git clone https://github.com/ComputeCanada/wheels_builder
# export PATH=$PATH:${{HOME}}/wheels_builder
# ### build KDEpy 1.1.0
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package KDEpy --version 1.1.0␣
 ↪--python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/packages/
# ### built nonconvexAG 1.0.6
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package nonconvexAG --version 1.
 ↪0.6 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/
# ### built fastHDMI 1.18.20
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package fastHDMI --version 1.18.
 ↪20 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/

# Here basically to build the packages at login node and install them in slurm␣
 ↪job submission locally
pip install --no-index bed-reader numpy sklearn matplotlib scipy numba␣
 ↪multiprocess scikit-learn cupy rpy2
pip install --no-index /home/kyang/KDEpy-1.1.
 ↪0+computecanada-cp38-cp38-linux_x86_64.whl
pip install --no-index /home/kyang/nonconvexAG-1.0.6+computecanada-py3-none-any.
 ↪whl
pip install --no-index /home/kyang/fastHDMI-1.18.20+computecanada-py3-none-any.
 ↪whl

nvidia-smi
lscpu

echo "running ABIDE_poly3_age_{dep_measure}_{fun_name}.py"

cp /home/kyang/ABIDE_data_analysis/ABIDE_PCA/ABIDE_PCA.csv $SLURM_TMPDIR/
cp ../ABIDE_columns.npy $SLURM_TMPDIR/
cp ../ABIDE_age_{dep_measure}_output.npy $SLURM_TMPDIR/
```

```
python3 ABIDE_poly3_age_{dep_measure}_{fun_name}.py
    """.format(dep_measure=dep_measure, fun_name=fun_name))
    py_script.write(r"""import numpy as np
import pandas as pd
from dask import dataframe as dd
import matplotlib.pyplot as plt
from scipy.stats import kendalltau, rankdata, norm
import fastHDMI as mi
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler, SplineTransformer
from sklearn.decomposition import PCA
from sklearn.linear_model import LassoCV, ElasticNetCV, RidgeCV, LarsCV,␣
 ↪LassoLarsCV, LogisticRegressionCV, LinearRegression, LogisticRegression
from sklearn.neural_network import MLPRegressor, MLPClassifier
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score, roc_auc_score
import multiprocess as mp
from tqdm import tqdm
import os

csv_file = os.environ["SLURM_TMPDIR"] + \
    r"/ABIDE_PCA.csv"
original_df = pd.read_csv(csv_file, encoding="unicode_escape", engine="c")

columns = np.load(os.environ["SLURM_TMPDIR"] + r"/ABIDE_columns.npy")
abide_dep = np.load(os.environ["SLURM_TMPDIR"] +
                    r"/ABIDE_age_{dep_measure}_output.npy")  # dep_measure
abide_dep = np.absolute(abide_dep)


def binning(var, num_bins, min_num=2):
    bins = np.linspace(np.min(var) - 1e-8, np.max(var) + 1e-8, num_bins)
    var_binned = np.digitize(var, bins)
    category = np.sort(np.unique(var_binned))
    while len([
            x for x in category if np.count_nonzero(var_binned == x) < min_num
    ]) != 0:
        for j in range(len(category)):
            if j < len(
                    category
            ):  # since category is always updated, we add this to avoid out of␣
 ↪index error; alternatively, a while loop also works
                if np.count_nonzero(
                        var_binned == category[j]
                ) < min_num:  # if the number of observations in a category is␣
 ↪less than min_num
```

```
                    if j == 0:  # if it's the first category, combine it with␣
 ↪the second
                        var_binned[var_binned == category[j]] = category[j + 1]
                    else:  # if it's not the first category, combine it with␣
 ↪the previous one
                        var_binned[var_binned == category[j]] = category[j - 1]
                    category = np.sort(np.unique(var_binned))
    return var_binned


def LogisticRegressionCV_l1(**arg):
    return LogisticRegressionCV(penalty="l1",
                                solver="saga",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_l2(**arg):
    return LogisticRegressionCV(penalty="l2",
                                solver="lbfgs",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_ElasticNet(**arg):
    return LogisticRegressionCV(penalty="elasticnet",
                                solver="saga",
                                multi_class="ovr",
                                l1_ratios=np.linspace(0, 1, 12)[1:-1],
                                **arg)


def testing_error(num_covariates=20,
                  training_proportion=.8,
                  fun=ElasticNetCV,
                  outcome_name="AGE_AT_SCAN",
                  seed=1):
    np.random.seed(seed)
    _usecols = np.hstack((
        outcome_name,  # "SEX", "DX_GROUP",
        columns[np.argsort(-abide_dep)][:num_covariates]))
    df = original_df[_usecols].dropna(inplace=False).sample(
        frac=1, random_state=seed, replace=False).reset_index(drop=True,
                                                              inplace=False)
    if df.shape[0] > 20:
        X, y = df.iloc[:,
                       1:].to_numpy(copy=True), df.iloc[:,
```

```
                                                    0].to_numpy(copy=True)
        X = StandardScaler(copy=False).fit_transform(X)
        X = SplineTransformer(n_knots=2,
                              degree=3,
                              extrapolation="continue",
                              include_bias=False).fit_transform(X)
        X = StandardScaler(copy=False).fit_transform(X)
        # if the outcome is continuous, we have to use binning
        if fun in [
                ElasticNetCV, LassoCV, RidgeCV, LarsCV, LassoLarsCV,
                MLPRegressor, RandomForestRegressor, LinearRegression
        ]:
            y_binned = binning(y, 30, min_num=2)
        else:
            y_binned = y.copy()
        X_train, X_test, y_train, y_test = train_test_split(
            X,
            y,
            train_size=training_proportion,
            random_state=seed,
            stratify=y_binned)
        if fun in [ElasticNetCV, LassoCV]:
            fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [RidgeCV]:  # RidgeCV doesn't have seed setting and n_jobs
            fit = fun(cv=5).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [LarsCV, LassoLarsCV
                     ]:  # LarsCV doesn't have seed setting but have n_jobs
            fit = fun(cv=5, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [MLPRegressor]:
            mlp_gs = fun(random_state=seed, max_iter=500)
            parameter_space = {{
                "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                       (500, )],
                "activation": ["tanh", "relu"],
                "solver": ["sgd", "adam"],
                "alpha": [0.0001, 0.05],
                "learning_rate": ["constant", "adaptive"]
            }}
            clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
            clf.fit(X_train, y_train)
            y_pred = clf.predict(X_test)
```

```
            out = r2_score(y_test, y_pred)
        elif fun in [MLPClassifier]:
            mlp_gs = fun(random_state=seed, max_iter=500)
            parameter_space = {{
                "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                       (500, )],
                "activation": ["tanh", "relu"],
                "solver": ["sgd", "adam"],
                "alpha": [0.0001, 0.05],
                "learning_rate": ["constant", "adaptive"]
            }}
            clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
            clf.fit(X_train, y_train)
            y_pred = clf.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [
                LogisticRegressionCV_l1, LogisticRegressionCV_l2,
                LogisticRegressionCV_ElasticNet
        ]:
            fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [RandomForestRegressor]:
            fit = fun(random_state=seed, n_jobs=10,
                      n_estimators=500).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [RandomForestClassifier]:
            fit = fun(random_state=seed, n_jobs=10,
                      n_estimators=500).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [LinearRegression]:
            fit = fun(n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [LogisticRegression]:
            fit = fun(penalty=None, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
    else:
        out = np.nan
    return out
```

```
def testing_error_rep(num_covariates=20,
                      training_proportion=.8,
                      fun=ElasticNetCV,
                      outcome_name="AGE_AT_SCAN",
                      num_rep=10):
    def _testing_error(seed):
        return testing_error(num_covariates=num_covariates,
                             training_proportion=training_proportion,
                             fun=fun,
                             outcome_name=outcome_name,
                             seed=seed)

    seeds = np.arange(num_rep)
    return np.array(list(map(_testing_error, seeds)))


def testing_error_num_attr(num_attr,
                           training_proportion=.8,
                           fun=ElasticNetCV,
                           outcome_name="AGE_AT_SCAN",
                           num_rep=10):
    def _testing_error_rep(_num_attr):
        return testing_error_rep(num_covariates=_num_attr,
                                 training_proportion=training_proportion,
                                 fun=fun,
                                 outcome_name=outcome_name,
                                 num_rep=num_rep)

    return np.array(list(map(_testing_error_rep, tqdm(num_attr))))


print(r"ABIDE_poly3_age_{dep_measure}_{fun_name}")  # dep_measure, fun_name
output = testing_error_num_attr(
    num_attr=list(map(int,
                      np.around(np.linspace(0, 50, 10 + 1)[1:]).tolist())),
    training_proportion=.8,  # 80/20 training+validation/testing division
    fun={fun_name},  # fun_name
    outcome_name="AGE_AT_SCAN",
    num_rep=20)
np.save(r"./ABIDE_poly3_age_{dep_measure}_{fun_name}",
        output)  # dep_measure, fun_name
    """.format(dep_measure=dep_measure, fun_name=fun_name))


dep_measure_list = []
```

```
for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]

for fun_name in [
        "LassoCV", "ElasticNetCV", "RidgeCV", "LarsCV", "LassoLarsCV",
        "MLPRegressor", "RandomForestRegressor", "LinearRegression"
]:
    for dep_measure in [*dep_measure_list, "Pearson", "skMI"]:
        job_creator(dep_measure, fun_name)
```

[10]:
```
#!find . -name "*.py" -exec yapf --in-place "{}" \;
#!find . -name "*.py" -exec autopep8 --in-place "{}" \;
# !find . -name "*.py" -exec yapf --in-place "{}" \;
# !find . -name "*.py" -exec autopep8 --in-place "{}" \;
```

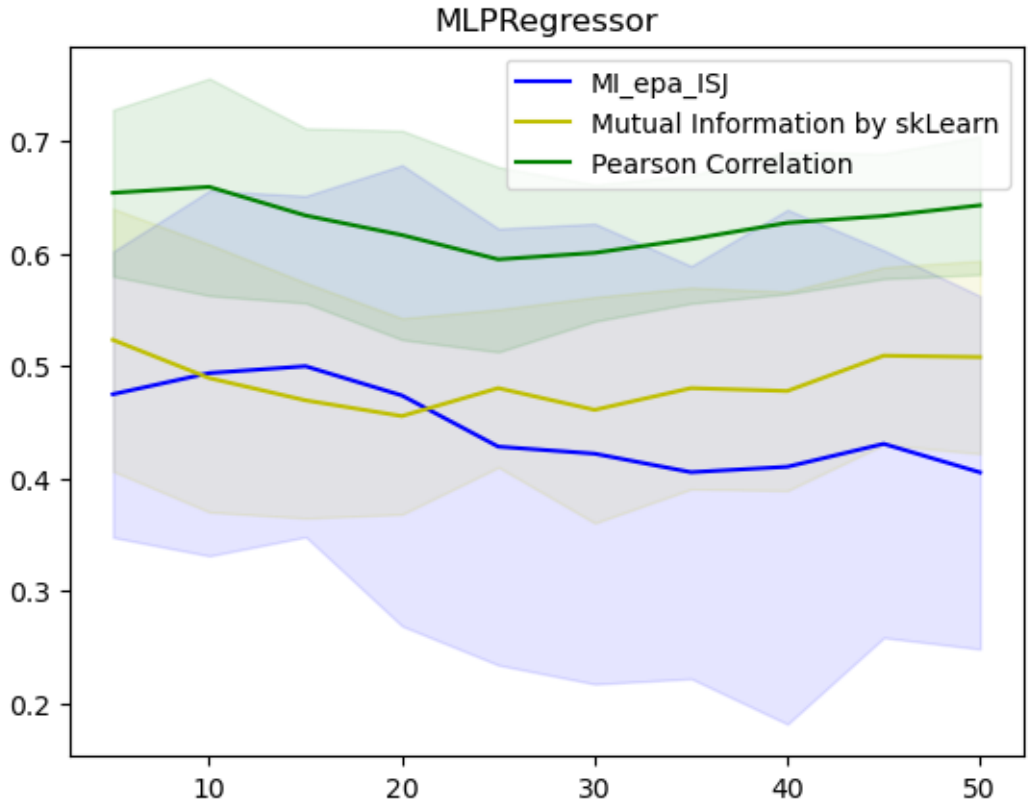
5 Comparison of Performance

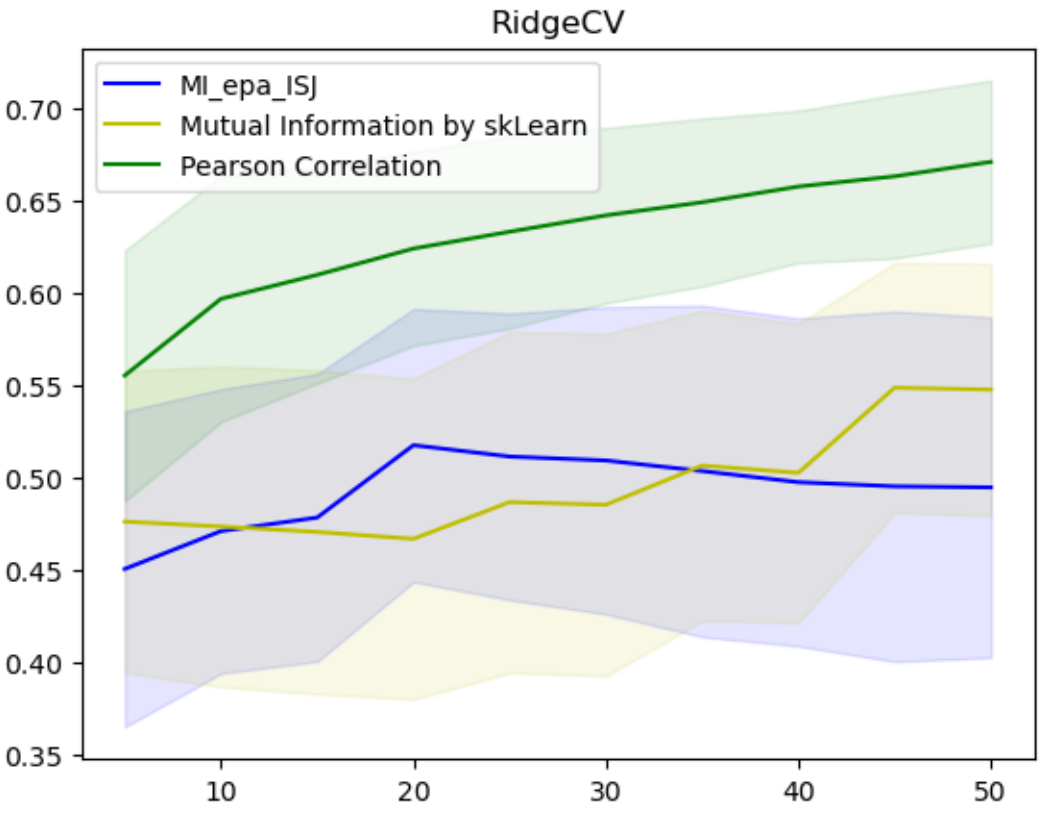
5.1 Here is just to show the testing set R^2

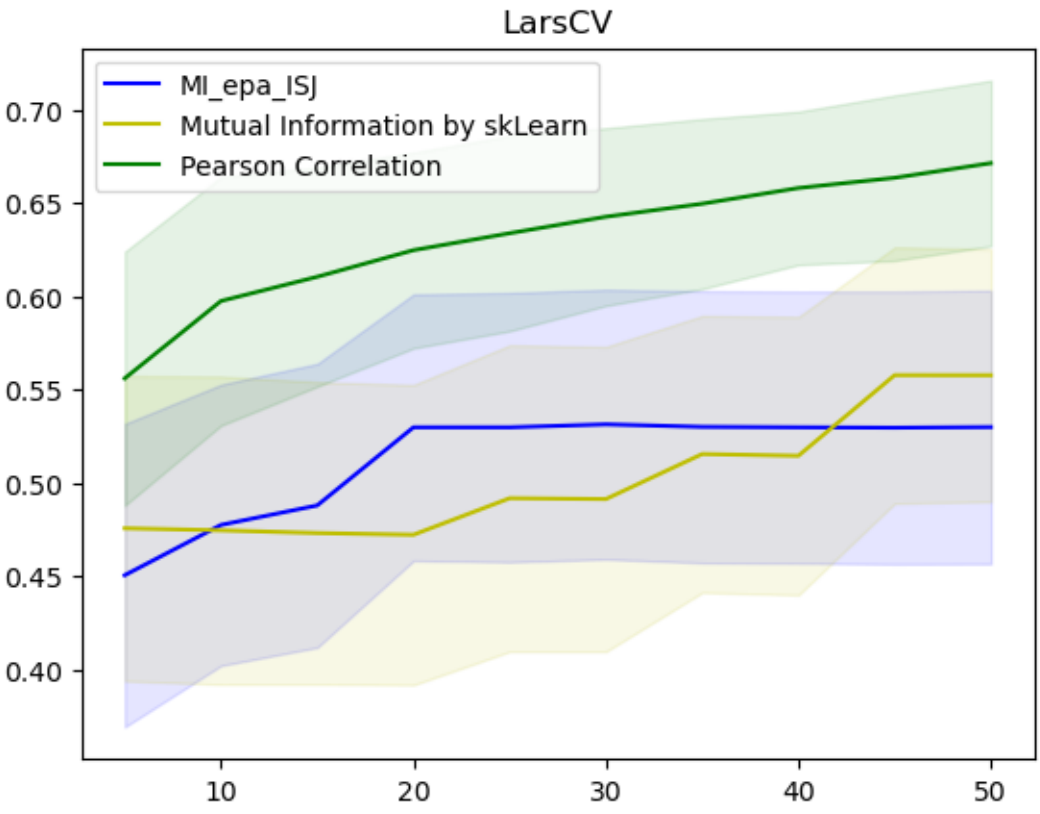
[11]:
```
import os


def plot_results(_plt, fun_name, dep_measure):
    if os.path.isfile(
            r"./ABIDE_predict_age/ABIDE_age_{dep_measure}_{fun_name}.npy".
            format(fun_name=fun_name, dep_measure=dep_measure)
    ) and os.path.isfile(
            r"./ABIDE_predict_age/ABIDE_age_skMI_{fun_name}.npy".
            format(fun_name=fun_name)) and os.path.isfile(
                r"./ABIDE_predict_age/ABIDE_age_Pearson_{fun_name}.npy".format(
                    fun_name=fun_name)):
        columns = np.load(r"./ABIDE_columns.npy")
        ABIDE_age_MI_foo = np.load(
            r"./ABIDE_predict_age/ABIDE_age_{dep_measure}_{fun_name}.npy".
            format(fun_name=fun_name, dep_measure=dep_measure))
        ABIDE_age_skMI_foo = np.load(
            r"./ABIDE_predict_age/ABIDE_age_skMI_{fun_name}.npy".format(
                fun_name=fun_name))
        ABIDE_age_Pearson_foo = np.load(
            r"./ABIDE_predict_age/ABIDE_age_Pearson_{fun_name}.npy".format(
                fun_name=fun_name))
        num_attr = list(
            map(int,
```

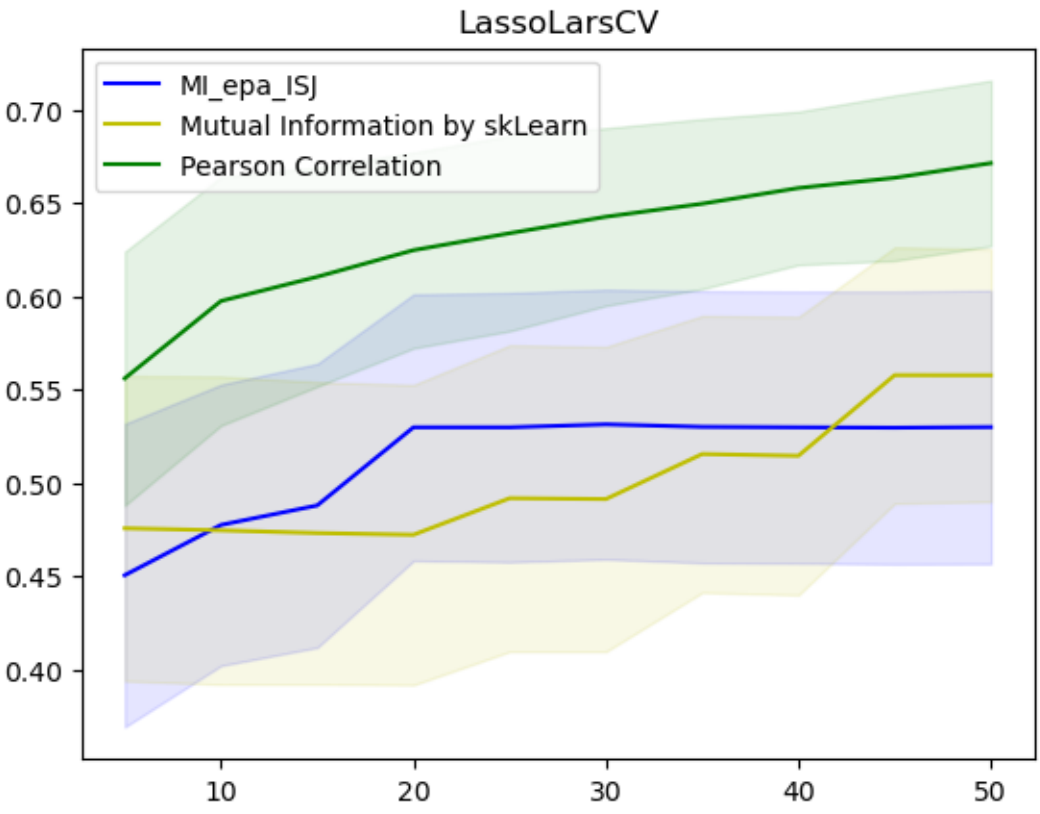
```
                np.around(np.linspace(
                    0, 50, 10 +
                    1)[1:]).tolist()))  # ADJUST this based on actual settings

        MI_fit_mean = np.mean(ABIDE_age_MI_foo, 1)
        MI_fit_std = np.std(ABIDE_age_MI_foo, 1)
        skMI_fit_mean = np.mean(ABIDE_age_skMI_foo, 1)
        skMI_fit_std = np.std(ABIDE_age_skMI_foo, 1)
        Pearson_fit_mean = np.mean(ABIDE_age_Pearson_foo, 1)
        Pearson_fit_std = np.std(ABIDE_age_Pearson_foo, 1)

        _plt.plot(num_attr, MI_fit_mean, label=dep_measure, color="b")
        _plt.fill_between(num_attr,
                          (MI_fit_mean + MI_fit_std * norm.ppf(0.025)),
                          (MI_fit_mean + MI_fit_std * norm.ppf(0.975)),
                          color="b",
                          alpha=.1)

        _plt.plot(num_attr,
                  skMI_fit_mean,
                  label="Mutual Information by skLearn",
                  color="y")
        _plt.fill_between(num_attr,
                          (skMI_fit_mean + skMI_fit_std * norm.ppf(0.025)),
                          (skMI_fit_mean + skMI_fit_std * norm.ppf(0.975)),
                          color="y",
                          alpha=.1)

        _plt.plot(num_attr,
                  Pearson_fit_mean,
                  label="Pearson Correlation",
                  color="g")
        _plt.fill_between(
            num_attr, (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.025)),
            (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.975)),
            color="g",
            alpha=.1)
        _plt.title(fun_name)
        _plt.legend()


dep_measure_list = []
for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
```

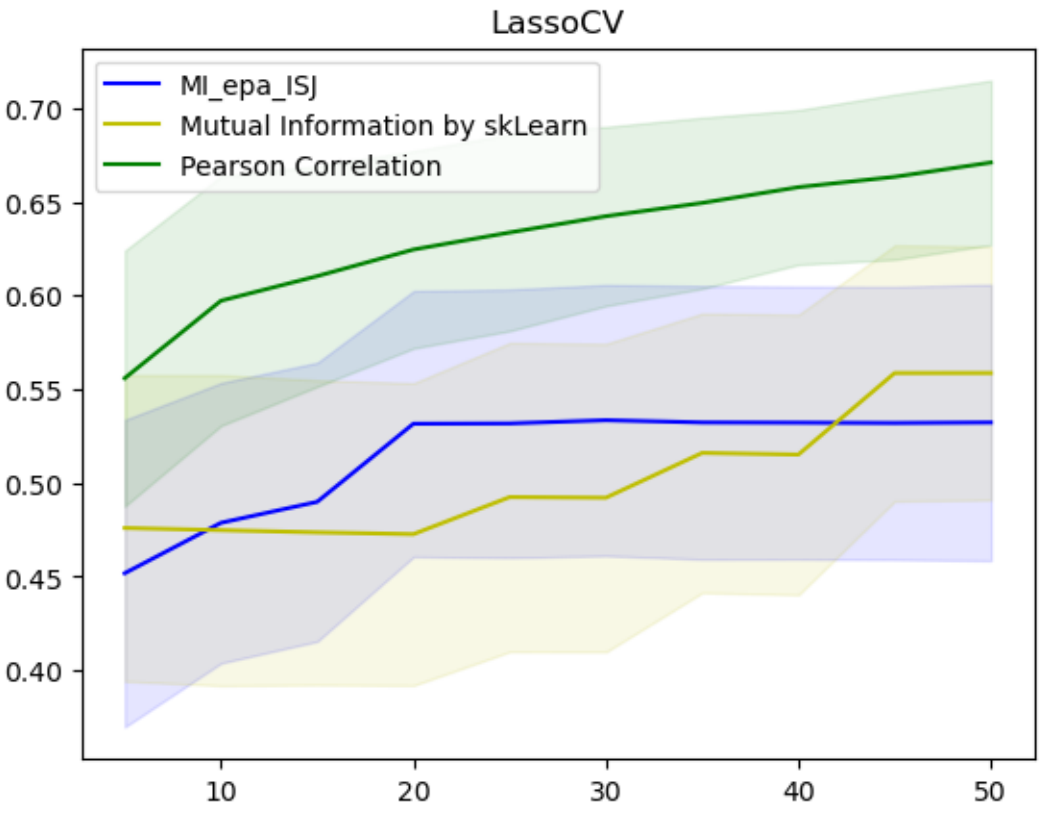
```
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]

for dep_measure in dep_measure_list:
    for fun_name in [
            "MLPRegressor", "RidgeCV", "LarsCV", "LassoLarsCV", "LassoCV",
            "ElasticNetCV", "RandomForestRegressor", "LinearRegression"
    ]:
        if dep_measure == "MI_epa_ISJ":
            plot_results(plt, fun_name, dep_measure=dep_measure)
            plt.savefig(r"./ABIDE_predict_age/" + fun_name + dep_measure)
            plt.show()
```

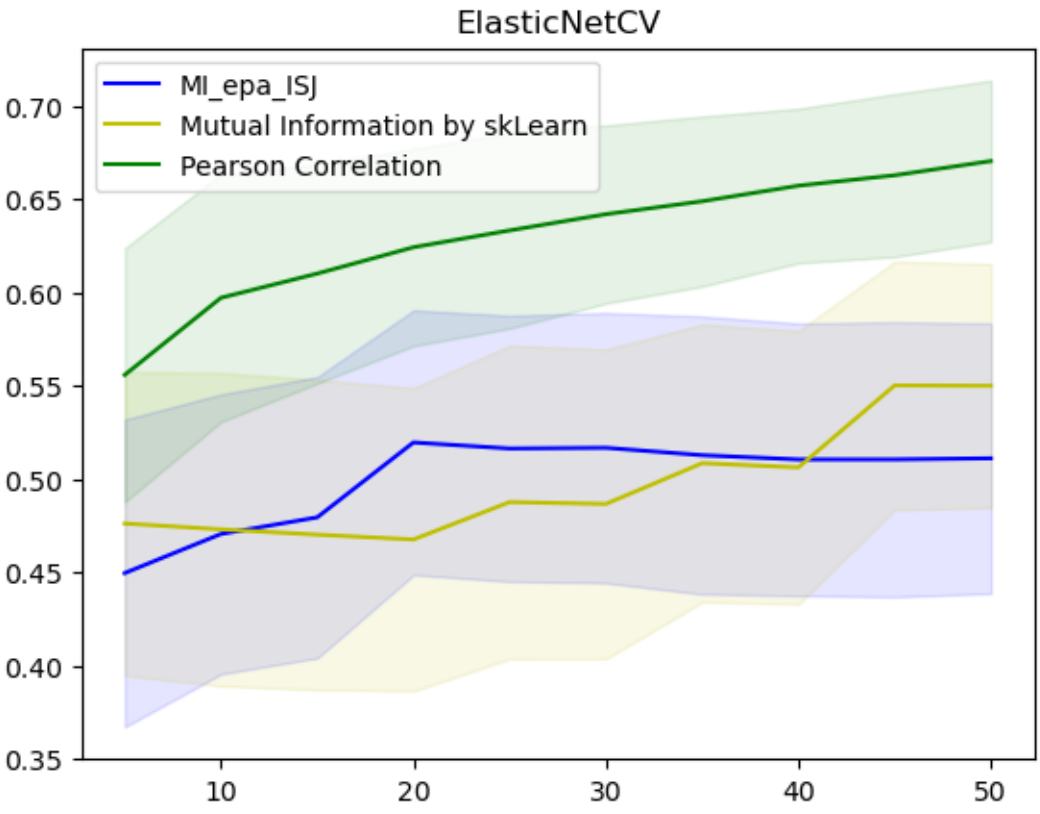


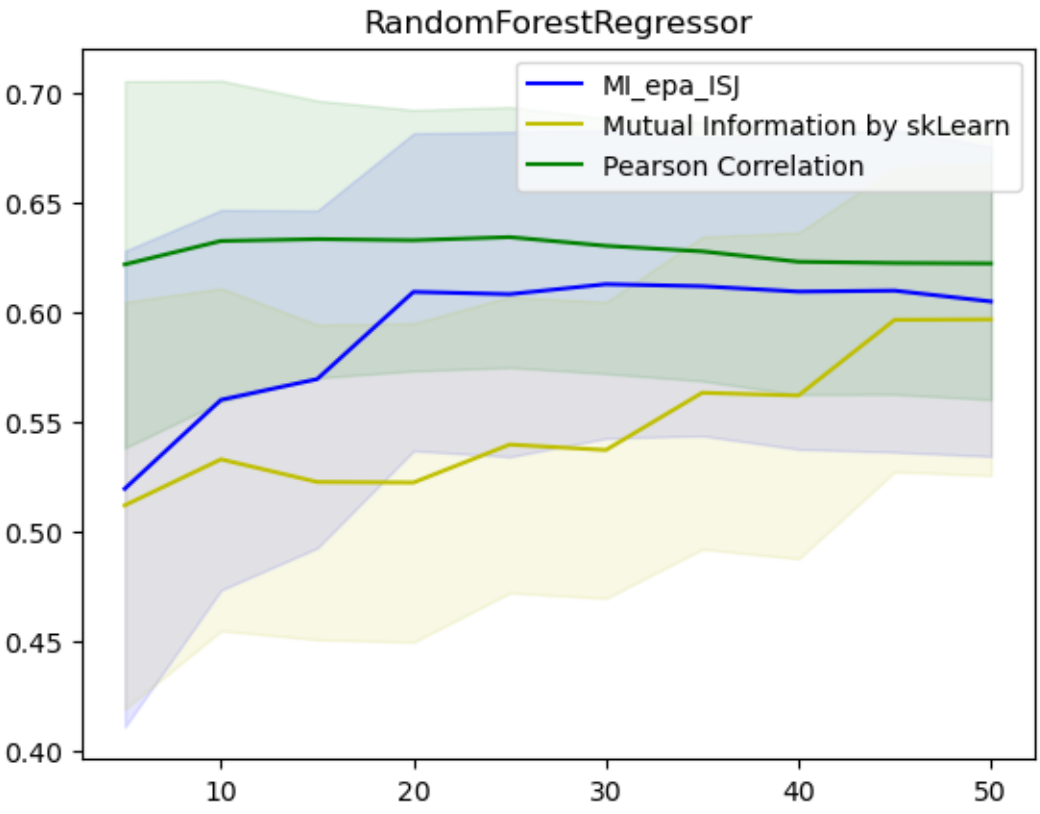

RidgeCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
10
20
30
40
50

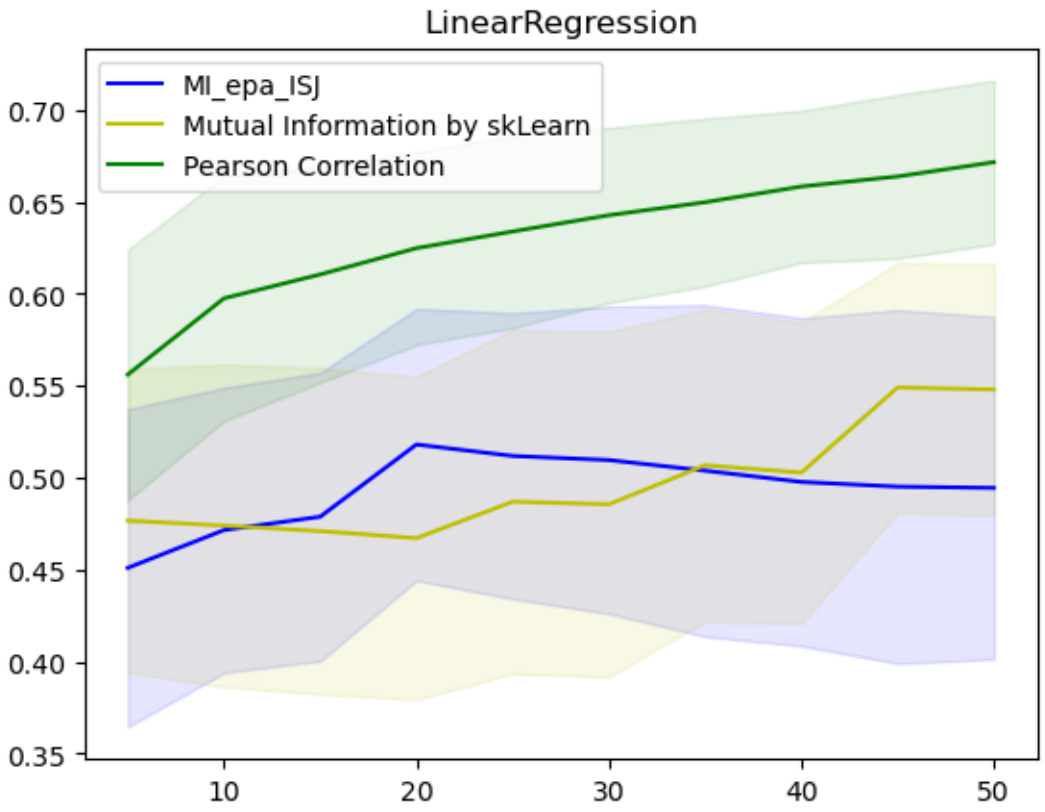

LarsCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
10
20
30
40
50


LassoLarsCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
10
20
30
40
50


LassoCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
10
20
30
40
50


ElasticNetCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
10
20
30
40
50

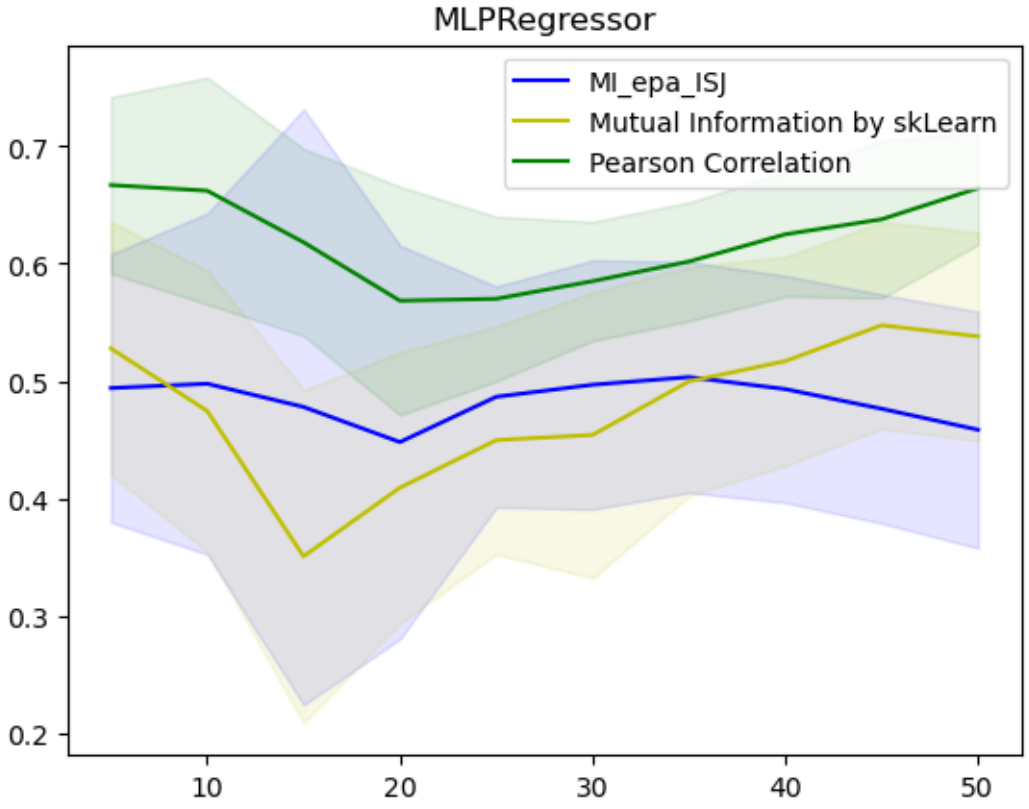

RandomForestRegressor
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
10
20
30
40
50

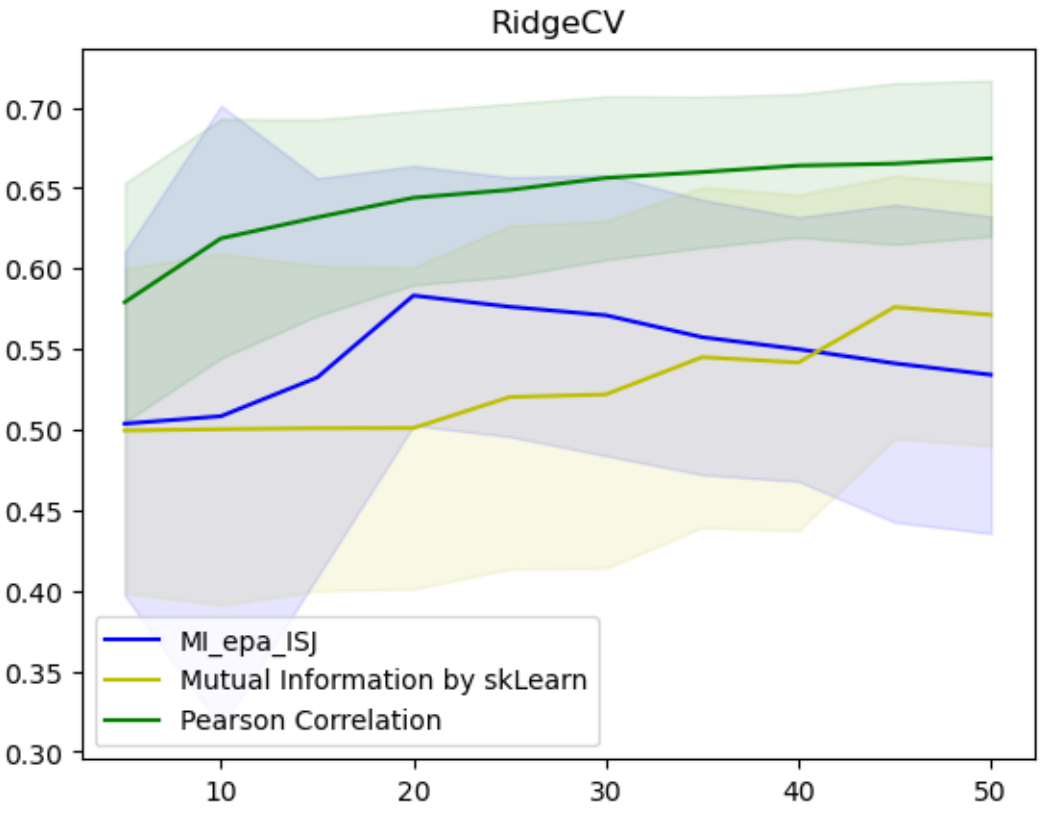


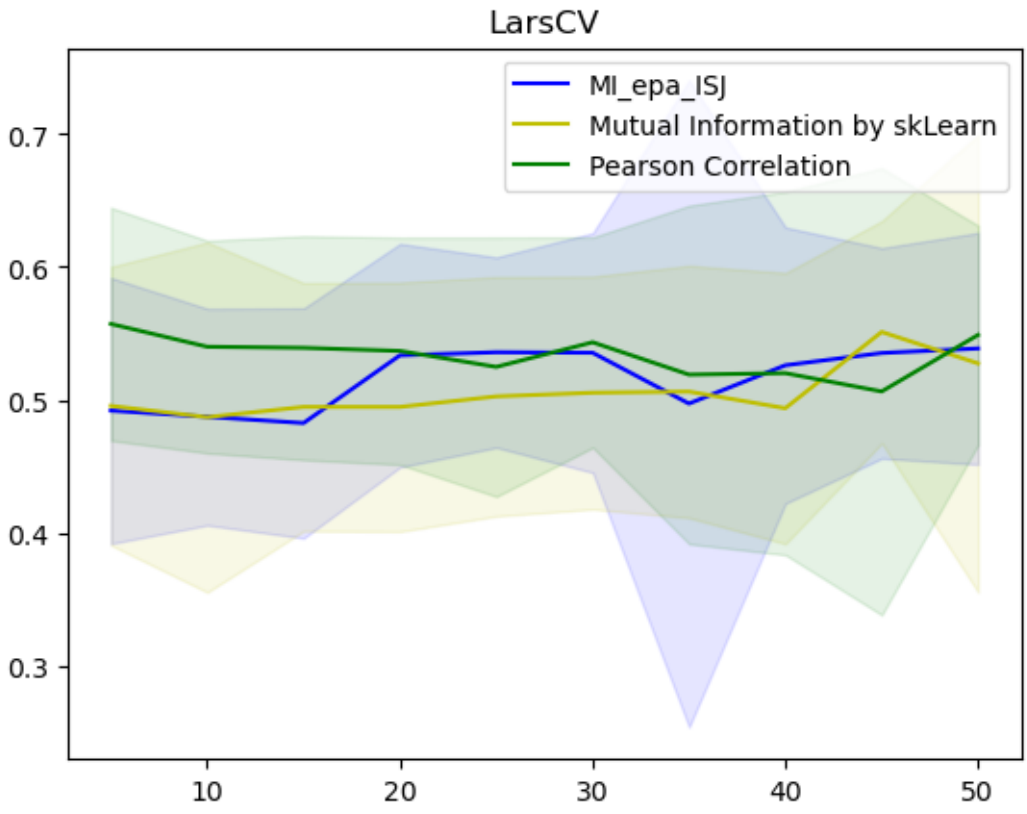
[12]:
```
import os


def plot_results(_plt, fun_name, dep_measure):
    if os.path.isfile(
            r"./ABIDE_poly3_predict_age/
 ↪ABIDE_poly3_age_{dep_measure}_{fun_name}.npy"
            .format(fun_name=fun_name, dep_measure=dep_measure)
    ) and os.path.isfile(
            r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_skMI_{fun_name}.npy".
            format(fun_name=fun_name)
    ) and os.path.isfile(
            r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_Pearson_{fun_name}.npy"
            .format(fun_name=fun_name)):
        columns = np.load(r"./ABIDE_columns.npy")
        ABIDE_age_MI_foo = np.load(
            r"./ABIDE_poly3_predict_age/
 ↪ABIDE_poly3_age_{dep_measure}_{fun_name}.npy"
            .format(fun_name=fun_name, dep_measure=dep_measure))
        ABIDE_age_skMI_foo = np.load(
            r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_skMI_{fun_name}.npy".
```

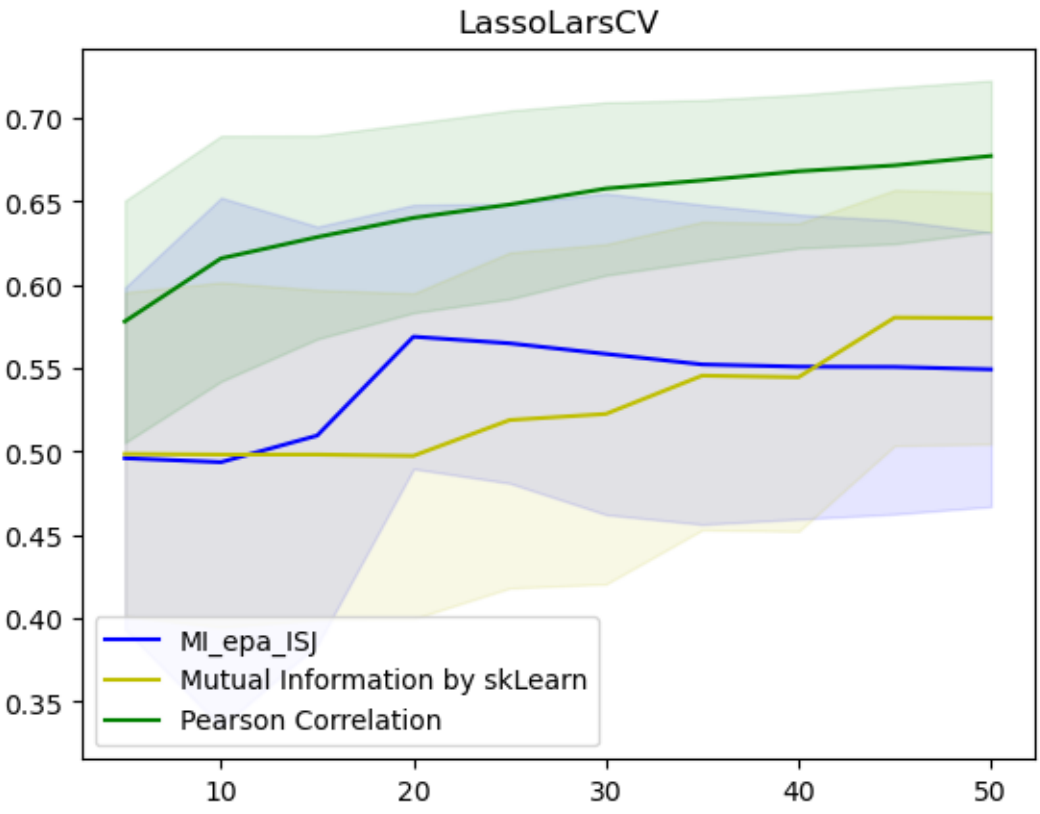
```
        format(fun_name=fun_name))
    ABIDE_age_Pearson_foo = np.load(
        r"./ABIDE_poly3_predict_age/ABIDE_poly3_age_Pearson_{fun_name}.npy"
        .format(fun_name=fun_name))
    num_attr = list(
        map(int,
            np.around(np.linspace(
                0, 50, 10 +
                1)[1:]).tolist()))  # ADJUST this based on actual settings

    MI_fit_mean = np.mean(ABIDE_age_MI_foo, 1)
    MI_fit_std = np.std(ABIDE_age_MI_foo, 1)
    skMI_fit_mean = np.mean(ABIDE_age_skMI_foo, 1)
    skMI_fit_std = np.std(ABIDE_age_skMI_foo, 1)
    Pearson_fit_mean = np.mean(ABIDE_age_Pearson_foo, 1)
    Pearson_fit_std = np.std(ABIDE_age_Pearson_foo, 1)

    _plt.plot(num_attr, MI_fit_mean, label=dep_measure, color="b")
    _plt.fill_between(num_attr,
                      (MI_fit_mean + MI_fit_std * norm.ppf(0.025)),
                      (MI_fit_mean + MI_fit_std * norm.ppf(0.975)),
                      color="b",
                      alpha=.1)

    _plt.plot(num_attr,
              skMI_fit_mean,
              label="Mutual Information by skLearn",
              color="y")
    _plt.fill_between(num_attr,
                      (skMI_fit_mean + skMI_fit_std * norm.ppf(0.025)),
                      (skMI_fit_mean + skMI_fit_std * norm.ppf(0.975)),
                      color="y",
                      alpha=.1)

    _plt.plot(num_attr,
              Pearson_fit_mean,
              label="Pearson Correlation",
              color="g")
    _plt.fill_between(
        num_attr, (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.025)),
        (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.975)),
        color="g",
        alpha=.1)
    _plt.title(fun_name)
    _plt.legend()
```

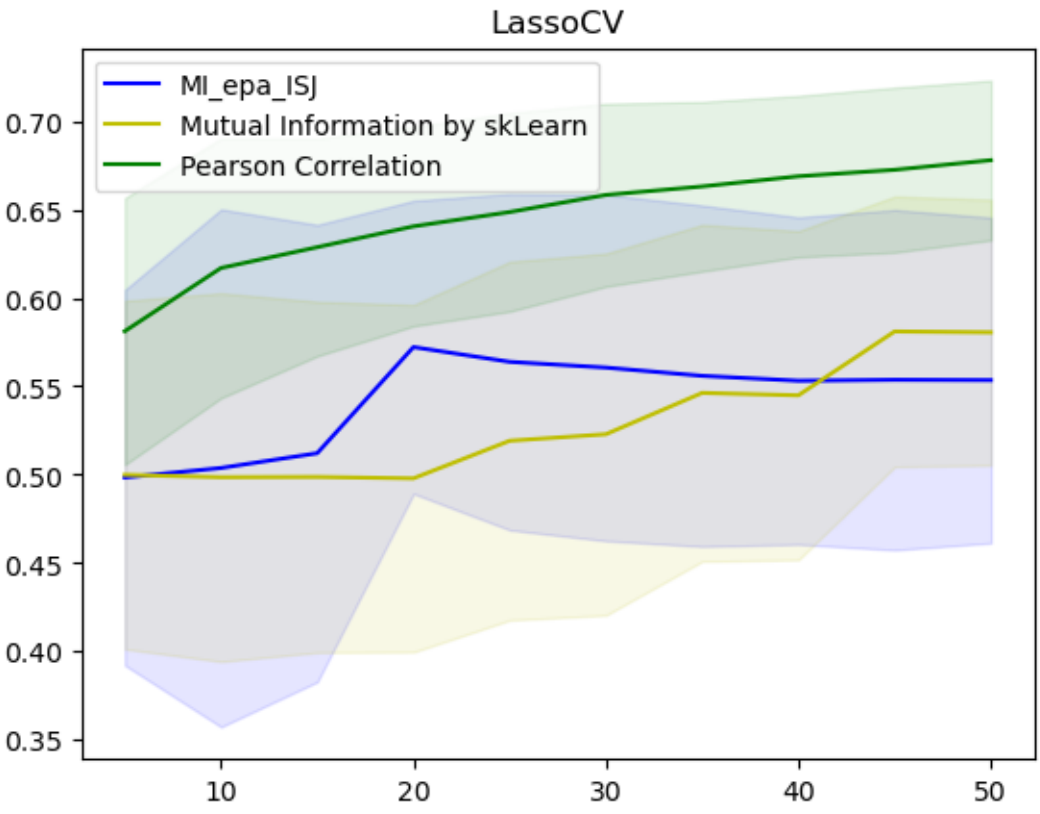
```
dep_measure_list = []
for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]

for dep_measure in dep_measure_list:
    for fun_name in [
            "MLPRegressor", "RidgeCV", "LarsCV", "LassoLarsCV", "LassoCV",
            "ElasticNetCV", "RandomForestRegressor", "LinearRegression"
    ]:
        if dep_measure == "MI_epa_ISJ":
            plot_results(plt, fun_name, dep_measure=dep_measure)
            plt.savefig(r"./ABIDE_poly3_predict_age/" + fun_name + dep_measure)
            plt.show()
```




RidgeCV
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
10
20
30
40
50
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation


LarsCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.7
0.6
0.5
0.4
0.3
10
20
30
40
50


LassoLarsCV
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
10
20
30
40
50
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation


LassoCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
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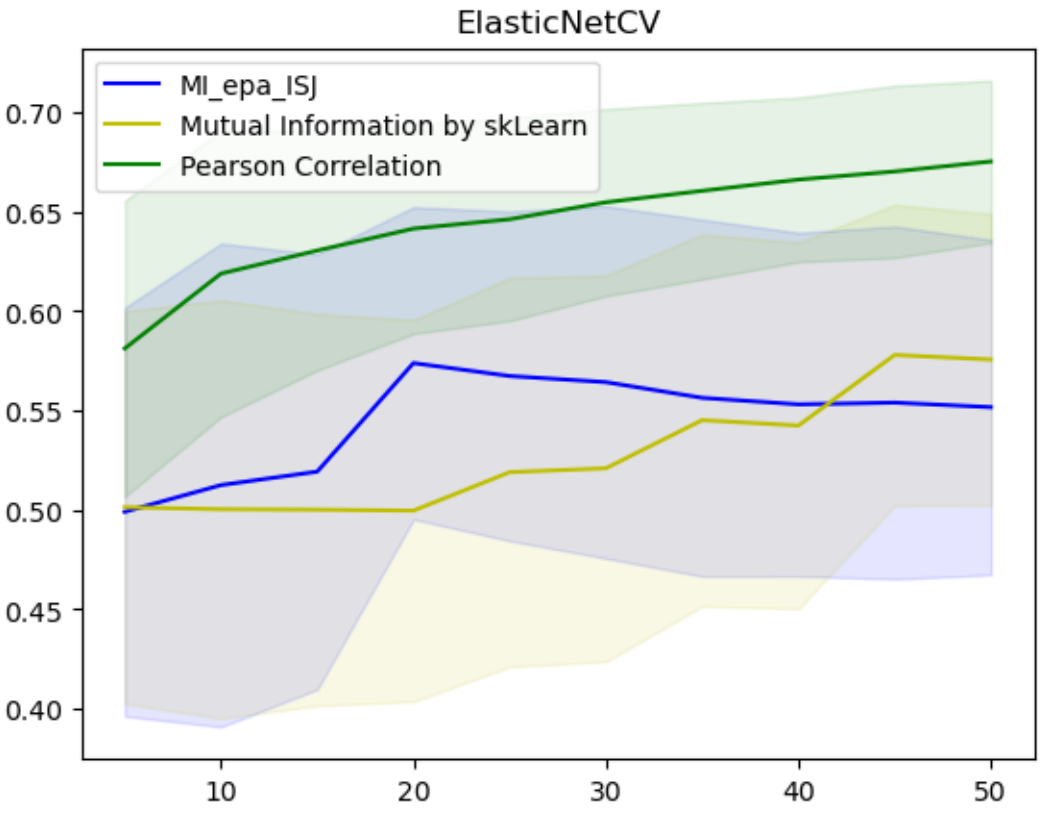
ElasticNetCV
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
0.40
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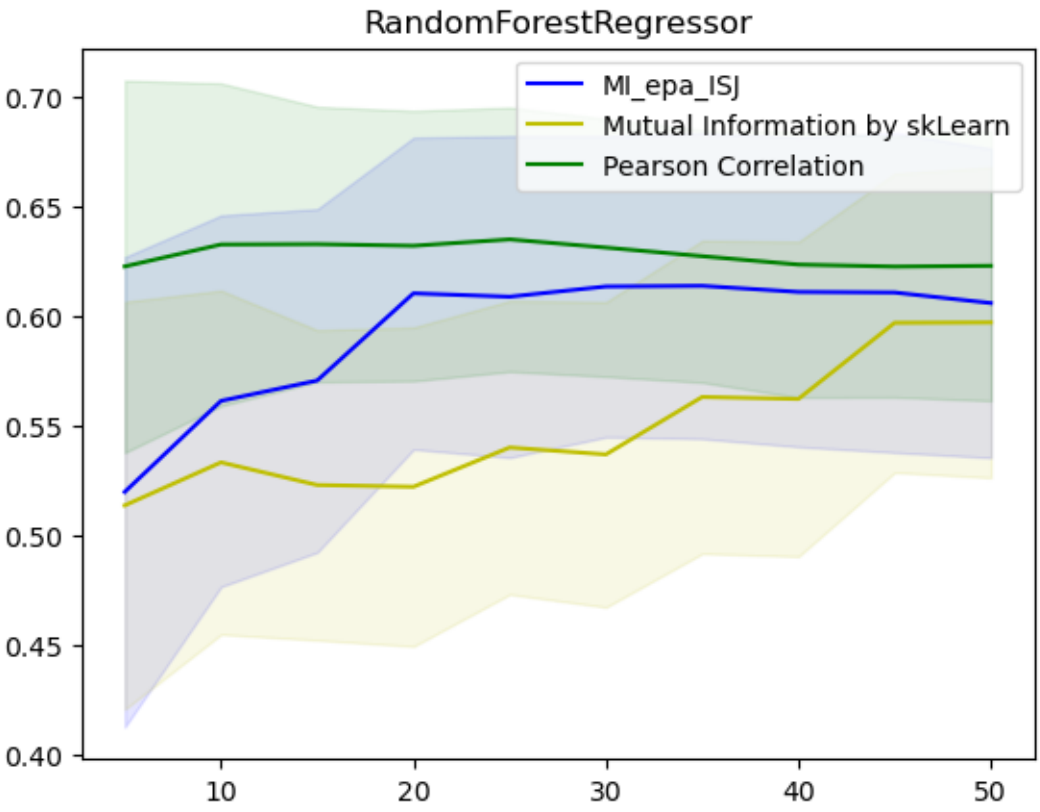
RandomForestRegressor
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.70
0.65
0.60
0.55
0.50
0.45
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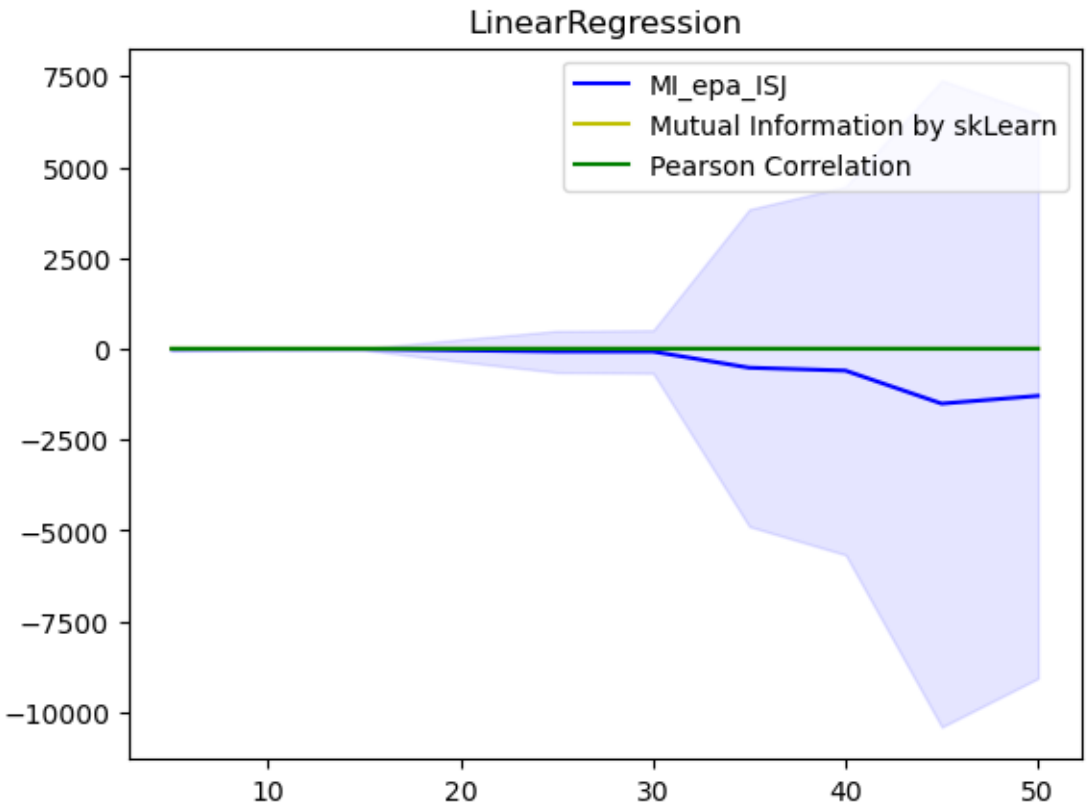


6 Try Fitting models to predict diagnosis, 5-fold CV

6.1 this block of code only means to be run on Compute Canada

6.1.1 ABIDE_predict_diagnosis

[13]:
```
from pathlib import Path


def job_creator(dep_measure, fun_name):
    Path(r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_" + dep_measure + "_" +
         fun_name + ".sh").touch()
    Path(r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_" + dep_measure + "_" +
         fun_name + ".py").touch()
    bash_script = open(
        r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_" + dep_measure + "_" +
        fun_name + ".sh", "w")
    py_script = open(
        r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_" + dep_measure + "_" +
        fun_name + ".py", "w")
    bash_script.write(r"""#!/bin/bash
```

```
#SBATCH --account=def-masd
#SBATCH --nodes=1
#SBATCH --cpus-per-task=10
#SBATCH --mem=80G
#SBATCH --time=3-12:00:00
#SBATCH --job-name=diagnosis_{dep_measure}_{fun_name}

module load gcc llvm rust arrow cuda nodejs python/3.8.10 r/4.0.2␣
 ↪python-build-bundle

virtualenv --no-download $SLURM_TMPDIR/env
source $SLURM_TMPDIR/env/bin/activate
pip install --no-index --upgrade pip

# ### run this block at the login node to build wheels
# ### get wheels builder
# git clone https://github.com/ComputeCanada/wheels_builder
# export PATH=$PATH:${{HOME}}/wheels_builder
# ### build KDEpy 1.1.0
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package KDEpy --version 1.1.0␣
 ↪--python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/packages/
# ### built nonconvexAG 1.0.6
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package nonconvexAG --version 1.
 ↪0.6 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/
# ### built fastHDMI 1.18.20
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package fastHDMI --version 1.18.
 ↪20 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/

# Here basically to build the packages at login node and install them in slurm␣
 ↪job submission locally
pip install --no-index bed-reader numpy sklearn matplotlib scipy numba␣
 ↪multiprocess scikit-learn cupy rpy2
pip install --no-index /home/kyang/KDEpy-1.1.
 ↪0+computecanada-cp38-cp38-linux_x86_64.whl
pip install --no-index /home/kyang/nonconvexAG-1.0.6+computecanada-py3-none-any.
 ↪whl
pip install --no-index /home/kyang/fastHDMI-1.18.20+computecanada-py3-none-any.
 ↪whl

nvidia-smi
lscpu

echo "running ABIDE_diagnosis_{dep_measure}_{fun_name}.py"
```

```
cp /home/kyang/ABIDE_data_analysis/ABIDE_PCA/ABIDE_PCA.csv $SLURM_TMPDIR/
cp ../ABIDE_columns.npy $SLURM_TMPDIR/
cp ../ABIDE_diagnosis_{dep_measure}_output.npy $SLURM_TMPDIR/

python3 ABIDE_diagnosis_{dep_measure}_{fun_name}.py
    """.format(dep_measure=dep_measure, fun_name=fun_name))
    py_script.write(r"""import numpy as np
import pandas as pd
from dask import dataframe as dd
import matplotlib.pyplot as plt
from scipy.stats import kendalltau, rankdata, norm
import fastHDMI as mi
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler, SplineTransformer
from sklearn.decomposition import PCA
from sklearn.linear_model import LassoCV, ElasticNetCV, RidgeCV, LarsCV,␣
 ↪LassoLarsCV, LogisticRegressionCV, LinearRegression, LogisticRegression
from sklearn.neural_network import MLPRegressor, MLPClassifier
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score, roc_auc_score
import multiprocess as mp
from tqdm import tqdm
import os

csv_file = os.environ["SLURM_TMPDIR"] + \
    r"/ABIDE_PCA.csv"
original_df = pd.read_csv(csv_file, encoding="unicode_escape", engine="c")

columns = np.load(os.environ["SLURM_TMPDIR"] + r"/ABIDE_columns.npy")
abide_dep = np.load(
    os.environ["SLURM_TMPDIR"] +
    r"/ABIDE_diagnosis_{dep_measure}_output.npy")  # dep_measure
abide_dep = np.absolute(abide_dep)


def binning(var, num_bins, min_num=2):
    bins = np.linspace(np.min(var) - 1e-8, np.max(var) + 1e-8, num_bins)
    var_binned = np.digitize(var, bins)
    category = np.sort(np.unique(var_binned))
    while len([
            x for x in category if np.count_nonzero(var_binned == x) < min_num
    ]) != 0:
        for j in range(len(category)):
            if j < len(
                    category
            ):  # since category is always updated, we add this to avoid out of␣
 ↪index error; alternatively, a while loop also works
```

```
                if np.count_nonzero(
                        var_binned == category[j]
                ) < min_num:  # if the number of observations in a category is␣
 ↪less than min_num
                    if j == 0:  # if it's the first category, combine it with␣
 ↪the second
                        var_binned[var_binned == category[j]] = category[j + 1]
                    else:  # if it's not the first category, combine it with␣
 ↪the previous one
                        var_binned[var_binned == category[j]] = category[j - 1]
                    category = np.sort(np.unique(var_binned))
    return var_binned


def LogisticRegressionCV_l1(**arg):
    return LogisticRegressionCV(penalty="l1",
                                solver="saga",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_l2(**arg):
    return LogisticRegressionCV(penalty="l2",
                                solver="lbfgs",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_ElasticNet(**arg):
    return LogisticRegressionCV(penalty="elasticnet",
                                solver="saga",
                                multi_class="ovr",
                                l1_ratios=np.linspace(0, 1, 12)[1:-1],
                                **arg)


def testing_error(num_covariates=20,
                  training_proportion=.8,
                  fun=ElasticNetCV,
                  outcome_name="AGE_AT_SCAN",
                  seed=1):
    np.random.seed(seed)
    _usecols = np.hstack((
        outcome_name,  # "SEX", "AGE_AT_SCAN",
        columns[np.argsort(-abide_dep)][:num_covariates]))
    df = original_df[_usecols].dropna(inplace=False).sample(
        frac=1, random_state=seed, replace=False).reset_index(drop=True,
```

```
                                                        inplace=False)
    if df.shape[0] > 20:
        X, y = df.iloc[:,
                       1:].to_numpy(copy=True), df.iloc[:,
                                                        0].to_numpy(copy=True)
        X = StandardScaler(copy=False).fit_transform(X)
        # if the outcome is continuous, we have to use binning
        if fun in [
                ElasticNetCV, LassoCV, RidgeCV, LarsCV, LassoLarsCV,
                MLPRegressor, RandomForestRegressor, LinearRegression
        ]:
            y_binned = binning(y, 30, min_num=2)
        else:
            y_binned = y.copy()
        X_train, X_test, y_train, y_test = train_test_split(
            X,
            y,
            train_size=training_proportion,
            random_state=seed,
            stratify=y_binned)
        if fun in [ElasticNetCV, LassoCV]:
            fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [RidgeCV]:  # RidgeCV doesn't have seed setting and n_jobs
            fit = fun(cv=5).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [LarsCV, LassoLarsCV
                     ]:  # LarsCV doesn't have seed setting but have n_jobs
            fit = fun(cv=5, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [MLPRegressor]:
            mlp_gs = fun(random_state=seed, max_iter=500)
            parameter_space = {{
                "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                       (500, )],
                "activation": ["tanh", "relu"],
                "solver": ["sgd", "adam"],
                "alpha": [0.0001, 0.05],
                "learning_rate": ["constant", "adaptive"]
            }}
            clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
            clf.fit(X_train, y_train)
            y_pred = clf.predict(X_test)
            out = r2_score(y_test, y_pred)
```

```
        elif fun in [MLPClassifier]:
            mlp_gs = fun(random_state=seed, max_iter=500)
            parameter_space = {{
                "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                       (500, )],
                "activation": ["tanh", "relu"],
                "solver": ["sgd", "adam"],
                "alpha": [0.0001, 0.05],
                "learning_rate": ["constant", "adaptive"]
            }}
            clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
            clf.fit(X_train, y_train)
            y_pred = clf.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [
                LogisticRegressionCV_l1, LogisticRegressionCV_l2,
                LogisticRegressionCV_ElasticNet
        ]:
            fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [RandomForestRegressor]:
            fit = fun(random_state=seed, n_jobs=10,
                      n_estimators=500).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [RandomForestClassifier]:
            fit = fun(random_state=seed, n_jobs=10,
                      n_estimators=500).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [LinearRegression]:
            fit = fun(n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [LogisticRegression]:
            fit = fun(penalty=None, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
    else:
        out = np.nan
    return out
```

```
def testing_error_rep(num_covariates=20,
                      training_proportion=.8,
                      fun=ElasticNetCV,
                      outcome_name="AGE_AT_SCAN",
                      num_rep=10):
    def _testing_error(seed):
        return testing_error(num_covariates=num_covariates,
                             training_proportion=training_proportion,
                             fun=fun,
                             outcome_name=outcome_name,
                             seed=seed)

    seeds = np.arange(num_rep)
    return np.array(list(map(_testing_error, seeds)))


def testing_error_num_attr(num_attr,
                           training_proportion=.8,
                           fun=ElasticNetCV,
                           outcome_name="AGE_AT_SCAN",
                           num_rep=10):
    def _testing_error_rep(_num_attr):
        return testing_error_rep(num_covariates=_num_attr,
                                 training_proportion=training_proportion,
                                 fun=fun,
                                 outcome_name=outcome_name,
                                 num_rep=num_rep)

    return np.array(list(map(_testing_error_rep, tqdm(num_attr))))


print(r"ABIDE_age_{dep_measure}_{fun_name}")  # dep_measure, fun_name
output = testing_error_num_attr(
    num_attr=list(map(int,
                      np.around(np.linspace(0, 50, 10 + 1)[1:]).tolist())),
    training_proportion=.8,  # 80/20 training+validation/testing division
    fun={fun_name},  # fun_name
    outcome_name="DX_GROUP",
    num_rep=20)
np.save(r"./ABIDE_diagnosis_{dep_measure}_{fun_name}",
        output)  # dep_measure, fun_name
    """.format(dep_measure=dep_measure, fun_name=fun_name))


dep_measure_list = []
for _kernel in [
```

```
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]

for fun_name in [
        "LogisticRegressionCV_l1", "LogisticRegressionCV_l2",
        "LogisticRegressionCV_ElasticNet", "MLPClassifier",
        "RandomForestClassifier", "LogisticRegression"
]:
    for dep_measure in [*dep_measure_list, "Pearson", "skMI"]:
        job_creator(dep_measure, fun_name)
```

[14]:
```
#!find . -name "*.py" -exec yapf --in-place "{}" \;
#!find . -name "*.py" -exec autopep8 --in-place "{}" \;
# !find . -name "*.py" -exec yapf --in-place "{}" \;
# !find . -name "*.py" -exec autopep8 --in-place "{}" \;
```

6.1.2 ABIDE_poly3_predict_diagnosis

[15]:
```
from pathlib import Path


def job_creator(dep_measure, fun_name):
    Path(r"./ABIDE_poly3_predict_diagnosis/ABIDE_poly3_diagnosis_" +
         dep_measure + "_" + fun_name + ".sh").touch()
    Path(r"./ABIDE_poly3_predict_diagnosis/ABIDE_poly3_diagnosis_" +
         dep_measure + "_" + fun_name + ".py").touch()
    bash_script = open(
        r"./ABIDE_poly3_predict_diagnosis/ABIDE_poly3_diagnosis_" +
        dep_measure + "_" + fun_name + ".sh", "w")
    py_script = open(
        r"./ABIDE_poly3_predict_diagnosis/ABIDE_poly3_diagnosis_" +
        dep_measure + "_" + fun_name + ".py", "w")
    bash_script.write(r"""#!/bin/bash
#SBATCH --account=def-cgreenwo
#SBATCH --nodes=1
#SBATCH --cpus-per-task=10
#SBATCH --mem=80G
#SBATCH --time=3-12:00:00
#SBATCH --job-name=poly3_diagnosis_{dep_measure}_{fun_name}

module load gcc llvm rust arrow cuda nodejs python/3.8.10 r/4.0.2␣
 ↪python-build-bundle

virtualenv --no-download $SLURM_TMPDIR/env
```

```
source $SLURM_TMPDIR/env/bin/activate
pip install --no-index --upgrade pip

# ### run this block at the login node to build wheels
# ### get wheels builder
# git clone https://github.com/ComputeCanada/wheels_builder
# export PATH=$PATH:${{HOME}}/wheels_builder
# ### build KDEpy 1.1.0
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package KDEpy --version 1.1.0␣
 ↪--python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/packages/
# ### built nonconvexAG 1.0.6
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package nonconvexAG --version 1.
 ↪0.6 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/
# ### built fastHDMI 1.18.20
# ${{HOME}}/wheels_builder/unmanylinuxize.sh --package fastHDMI --version 1.18.
 ↪20 --python 3.8,3.9,3.10 --find_links https://files.pythonhosted.org/
 ↪packages/

# Here basically to build the packages at login node and install them in slurm␣
 ↪job submission locally
pip install --no-index bed-reader numpy sklearn matplotlib scipy numba␣
 ↪multiprocess scikit-learn cupy rpy2
pip install --no-index /home/kyang/KDEpy-1.1.
 ↪0+computecanada-cp38-cp38-linux_x86_64.whl
pip install --no-index /home/kyang/nonconvexAG-1.0.6+computecanada-py3-none-any.
 ↪whl
pip install --no-index /home/kyang/fastHDMI-1.18.20+computecanada-py3-none-any.
 ↪whl

nvidia-smi
lscpu

echo "running ABIDE_poly3_diagnosis_{dep_measure}_{fun_name}.py"

cp /home/kyang/ABIDE_data_analysis/ABIDE_PCA/ABIDE_PCA.csv $SLURM_TMPDIR/
cp ../ABIDE_columns.npy $SLURM_TMPDIR/
cp ../ABIDE_diagnosis_{dep_measure}_output.npy $SLURM_TMPDIR/

python3 ABIDE_poly3_diagnosis_{dep_measure}_{fun_name}.py
    """.format(dep_measure=dep_measure, fun_name=fun_name))
    py_script.write(r"""import numpy as np
import pandas as pd
from dask import dataframe as dd
import matplotlib.pyplot as plt
from scipy.stats import kendalltau, rankdata, norm
```

```
import fastHDMI as mi
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler, SplineTransformer
from sklearn.decomposition import PCA
from sklearn.linear_model import LassoCV, ElasticNetCV, RidgeCV, LarsCV,␣
 ↪LassoLarsCV, LogisticRegressionCV, LinearRegression, LogisticRegression
from sklearn.neural_network import MLPRegressor, MLPClassifier
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score, roc_auc_score
import multiprocess as mp
from tqdm import tqdm
import os

csv_file = os.environ["SLURM_TMPDIR"] + \
    r"/ABIDE_PCA.csv"
original_df = pd.read_csv(csv_file, encoding="unicode_escape", engine="c")

columns = np.load(os.environ["SLURM_TMPDIR"] + r"/ABIDE_columns.npy")
abide_dep = np.load(
    os.environ["SLURM_TMPDIR"] +
    r"/ABIDE_diagnosis_{dep_measure}_output.npy")  # dep_measure
abide_dep = np.absolute(abide_dep)


def binning(var, num_bins, min_num=2):
    bins = np.linspace(np.min(var) - 1e-8, np.max(var) + 1e-8, num_bins)
    var_binned = np.digitize(var, bins)
    category = np.sort(np.unique(var_binned))
    while len([
            x for x in category if np.count_nonzero(var_binned == x) < min_num
    ]) != 0:
        for j in range(len(category)):
            if j < len(
                    category
            ):  # since category is always updated, we add this to avoid out of␣
 ↪index error; alternatively, a while loop also works
                if np.count_nonzero(
                        var_binned == category[j]
                ) < min_num:  # if the number of observations in a category is␣
 ↪less than min_num
                    if j == 0:  # if it's the first category, combine it with␣
 ↪the second
                        var_binned[var_binned == category[j]] = category[j + 1]
                    else:  # if it's not the first category, combine it with␣
 ↪the previous one
                        var_binned[var_binned == category[j]] = category[j - 1]
                    category = np.sort(np.unique(var_binned))
```

```
    return var_binned


def LogisticRegressionCV_l1(**arg):
    return LogisticRegressionCV(penalty="l1",
                                solver="saga",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_l2(**arg):
    return LogisticRegressionCV(penalty="l2",
                                solver="lbfgs",
                                multi_class="ovr",
                                **arg)


def LogisticRegressionCV_ElasticNet(**arg):
    return LogisticRegressionCV(penalty="elasticnet",
                                solver="saga",
                                multi_class="ovr",
                                l1_ratios=np.linspace(0, 1, 12)[1:-1],
                                **arg)


def testing_error(num_covariates=20,
                  training_proportion=.8,
                  fun=ElasticNetCV,
                  outcome_name="AGE_AT_SCAN",
                  seed=1):
    np.random.seed(seed)
    _usecols = np.hstack((
        outcome_name,  # "SEX", "AGE_AT_SCAN",
        columns[np.argsort(-abide_dep)][:num_covariates]))
    df = original_df[_usecols].dropna(inplace=False).sample(
        frac=1, random_state=seed, replace=False).reset_index(drop=True,
                                                              inplace=False)
    if df.shape[0] > 20:
        X, y = df.iloc[:,
                       1:].to_numpy(copy=True), df.iloc[:,
                                                        0].to_numpy(copy=True)
        X = StandardScaler(copy=False).fit_transform(X)
        X = SplineTransformer(n_knots=2,
                              degree=3,
                              extrapolation="continue",
                              include_bias=False).fit_transform(X)
        X = StandardScaler(copy=False).fit_transform(X)
```

```
        # if the outcome is continuous, we have to use binning
        if fun in [
                ElasticNetCV, LassoCV, RidgeCV, LarsCV, LassoLarsCV,
                MLPRegressor, RandomForestRegressor, LinearRegression
        ]:
            y_binned = binning(y, 30, min_num=2)
        else:
            y_binned = y.copy()
        X_train, X_test, y_train, y_test = train_test_split(
            X,
            y,
            train_size=training_proportion,
            random_state=seed,
            stratify=y_binned)
        if fun in [ElasticNetCV, LassoCV]:
            fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [RidgeCV]:  # RidgeCV doesn't have seed setting and n_jobs
            fit = fun(cv=5).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [LarsCV, LassoLarsCV
                     ]:  # LarsCV doesn't have seed setting but have n_jobs
            fit = fun(cv=5, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [MLPRegressor]:
            mlp_gs = fun(random_state=seed, max_iter=500)
            parameter_space = {{
                "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                       (500, )],
                "activation": ["tanh", "relu"],
                "solver": ["sgd", "adam"],
                "alpha": [0.0001, 0.05],
                "learning_rate": ["constant", "adaptive"]
            }}
            clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
            clf.fit(X_train, y_train)
            y_pred = clf.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [MLPClassifier]:
            mlp_gs = fun(random_state=seed, max_iter=500)
            parameter_space = {{
                "hidden_layer_sizes": [(15, 15, 15, 15, 15, 15), (30, 20, 20),
                                       (500, )],
                "activation": ["tanh", "relu"],
```

```
                "solver": ["sgd", "adam"],
                "alpha": [0.0001, 0.05],
                "learning_rate": ["constant", "adaptive"]
            }}
            clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=10, cv=5)
            clf.fit(X_train, y_train)
            y_pred = clf.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [
                LogisticRegressionCV_l1, LogisticRegressionCV_l2,
                LogisticRegressionCV_ElasticNet
        ]:
            fit = fun(cv=5, random_state=seed, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [RandomForestRegressor]:
            fit = fun(random_state=seed, n_jobs=10,
                      n_estimators=500).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [RandomForestClassifier]:
            fit = fun(random_state=seed, n_jobs=10,
                      n_estimators=500).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
        elif fun in [LinearRegression]:
            fit = fun(n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict(X_test)
            out = r2_score(y_test, y_pred)
        elif fun in [LogisticRegression]:
            fit = fun(penalty=None, n_jobs=10).fit(X_train, y_train)
            y_pred = fit.predict_proba(
                X_test)[:, 1]  # predict probability to calculate ROC
            out = roc_auc_score(y_test, y_pred)
    else:
        out = np.nan
    return out


def testing_error_rep(num_covariates=20,
                      training_proportion=.8,
                      fun=ElasticNetCV,
                      outcome_name="AGE_AT_SCAN",
                      num_rep=10):
```

```
    def _testing_error(seed):
        return testing_error(num_covariates=num_covariates,
                             training_proportion=training_proportion,
                             fun=fun,
                             outcome_name=outcome_name,
                             seed=seed)

    seeds = np.arange(num_rep)
    return np.array(list(map(_testing_error, seeds)))


def testing_error_num_attr(num_attr,
                           training_proportion=.8,
                           fun=ElasticNetCV,
                           outcome_name="AGE_AT_SCAN",
                           num_rep=10):
    def _testing_error_rep(_num_attr):
        return testing_error_rep(num_covariates=_num_attr,
                                 training_proportion=training_proportion,
                                 fun=fun,
                                 outcome_name=outcome_name,
                                 num_rep=num_rep)

    return np.array(list(map(_testing_error_rep, tqdm(num_attr))))


print(r"ABIDE_poly3_age_{dep_measure}_{fun_name}")  # dep_measure, fun_name
output = testing_error_num_attr(
    num_attr=list(map(int,
                      np.around(np.linspace(0, 50, 10 + 1)[1:]).tolist())),
    training_proportion=.8,  # 80/20 training+validation/testing division
    fun={fun_name},  # fun_name
    outcome_name="DX_GROUP",
    num_rep=20)
np.save(r"./ABIDE_poly3_diagnosis_{dep_measure}_{fun_name}",
        output)  # dep_measure, fun_name
    """.format(dep_measure=dep_measure, fun_name=fun_name))


dep_measure_list = []
for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]
```

```
for fun_name in [
        "LogisticRegressionCV_l1", "LogisticRegressionCV_l2",
        "LogisticRegressionCV_ElasticNet", "MLPClassifier",
        "RandomForestClassifier", "LogisticRegression"
]:
    for dep_measure in [*dep_measure_list, "Pearson", "skMI"]:
        job_creator(dep_measure, fun_name)
```

[16]:
```
#!find . -name "*.py" -exec yapf --in-place "{}" \;
#!find . -name "*.py" -exec autopep8 --in-place "{}" \;
!find . -name "*.py" -exec yapf --in-place "{}" \;
!find . -name "*.py" -exec autopep8 --in-place "{}" \;
```

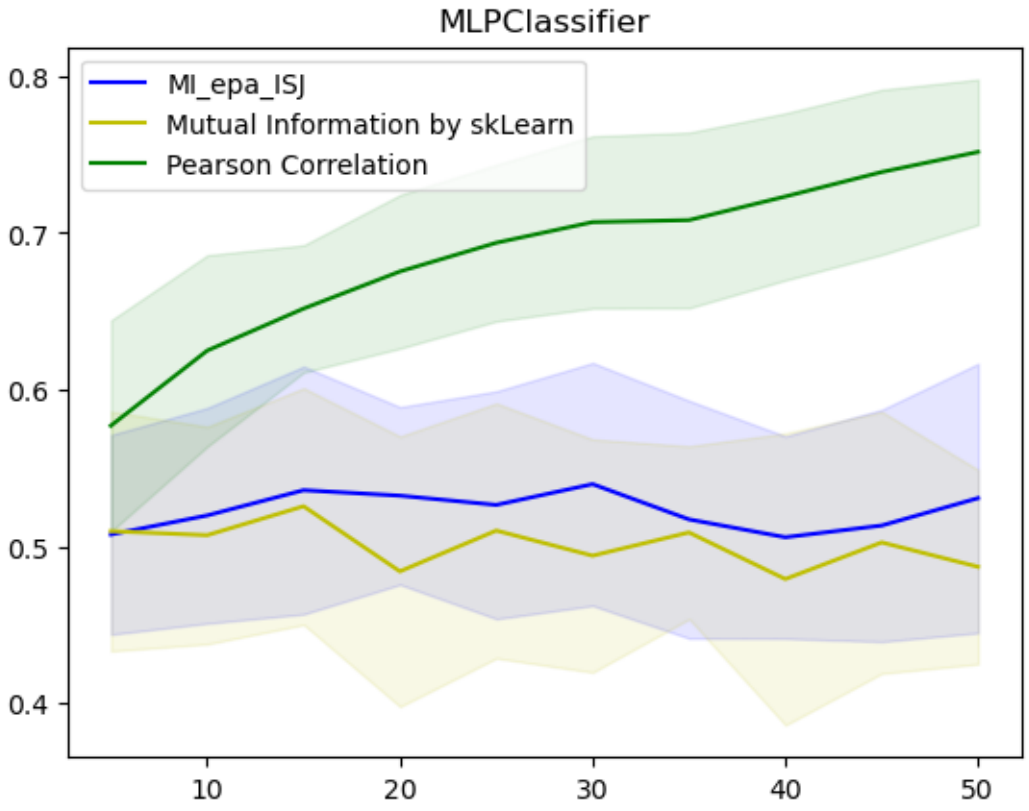
7 Comparison of Performance

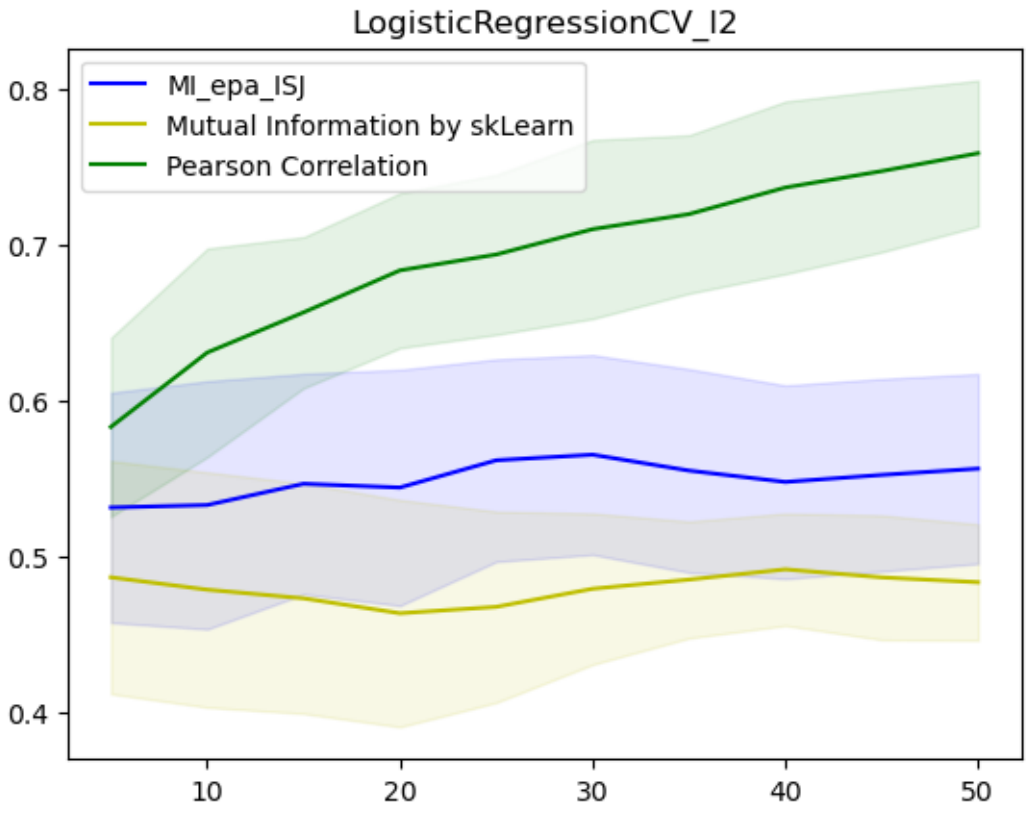
7.1 Here is just to show the testing set ROC

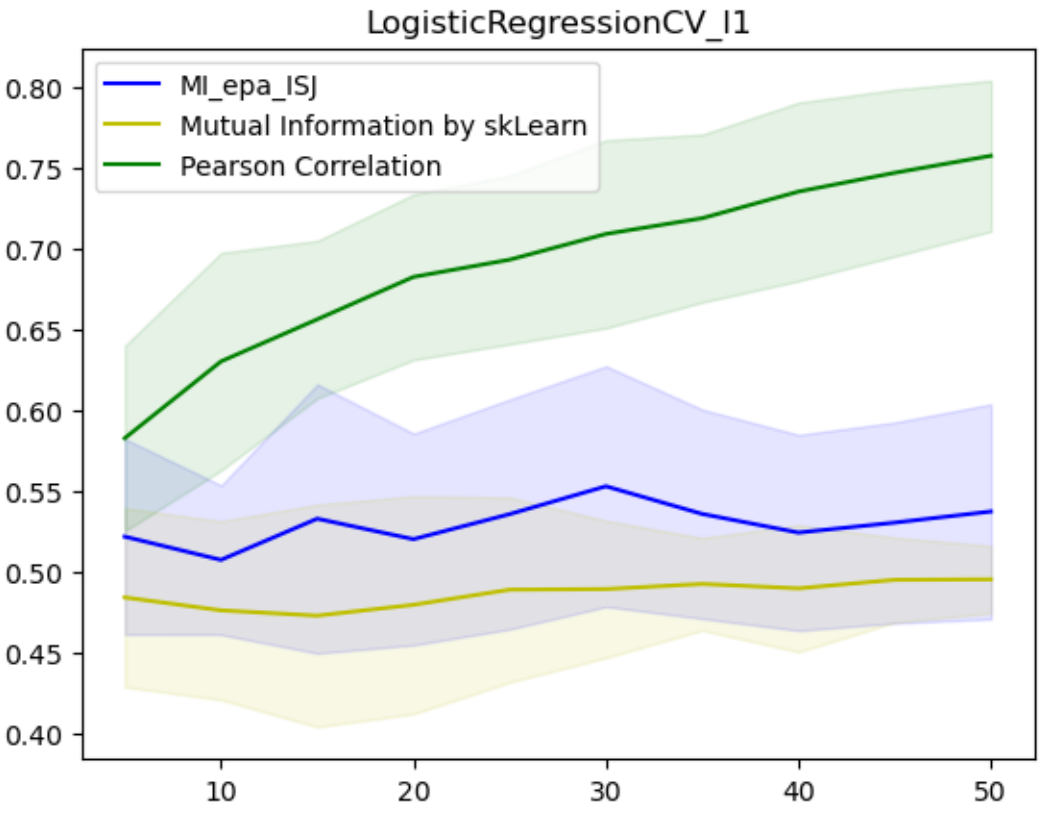
[17]:
```
import os


def plot_results(_plt, fun_name, dep_measure):
    if os.path.isfile(
            r"./ABIDE_predict_diagnosis/
 ↪ABIDE_diagnosis_{dep_measure}_{fun_name}.npy"
            .format(fun_name=fun_name, dep_measure=dep_measure)
    ) and os.path.isfile(
            r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_skMI_{fun_name}.npy".
            format(fun_name=fun_name)
    ) and os.path.isfile(
            r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_Pearson_{fun_name}.npy"
            .format(fun_name=fun_name)):
        columns = np.load(r"./ABIDE_columns.npy")
        ABIDE_diagnosis_MI_foo = np.load(
            r"./ABIDE_predict_diagnosis/
 ↪ABIDE_diagnosis_{dep_measure}_{fun_name}.npy"
            .format(fun_name=fun_name, dep_measure=dep_measure))
        ABIDE_diagnosis_skMI_foo = np.load(
            r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_skMI_{fun_name}.npy".
            format(fun_name=fun_name))
        ABIDE_diagnosis_Pearson_foo = np.load(
            r"./ABIDE_predict_diagnosis/ABIDE_diagnosis_Pearson_{fun_name}.npy"
            .format(fun_name=fun_name))
        num_attr = list(
            map(int,
                np.around(np.linspace(
                    0, 50, 10 +
                    1)[1:]).tolist()))  # ADJUST this based on actual settings
```

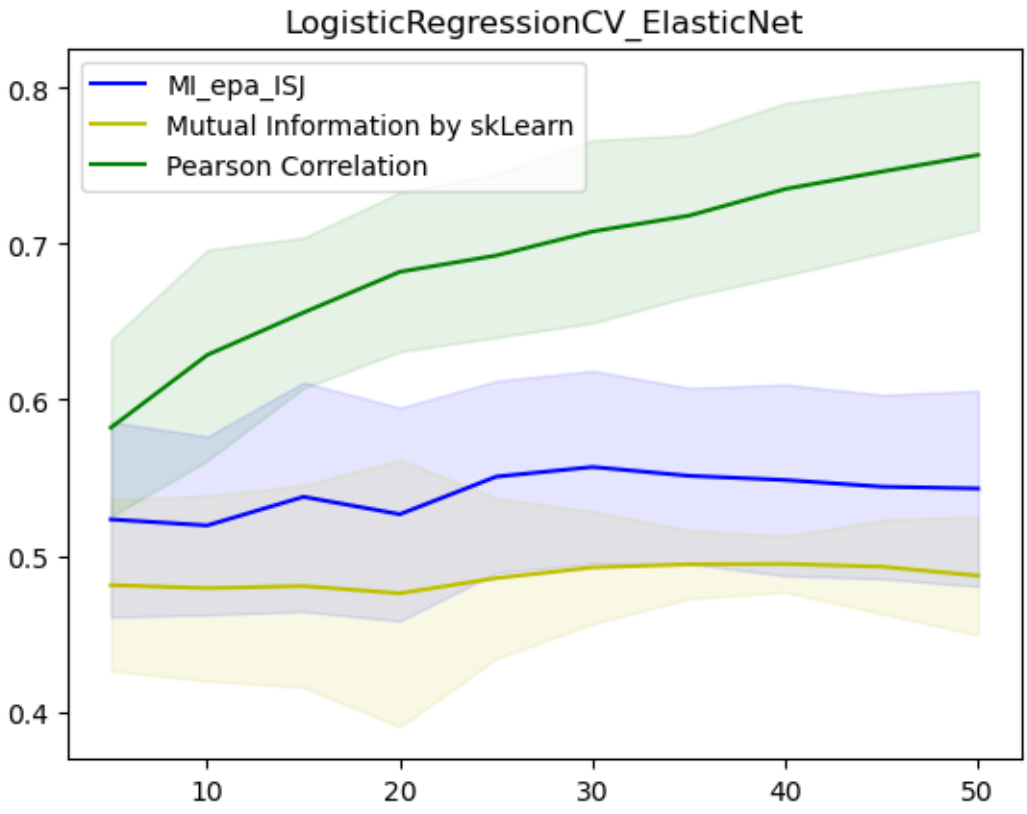
```
        MI_fit_mean = np.mean(ABIDE_diagnosis_MI_foo, 1)
        MI_fit_std = np.std(ABIDE_diagnosis_MI_foo, 1)
        skMI_fit_mean = np.mean(ABIDE_diagnosis_skMI_foo, 1)
        skMI_fit_std = np.std(ABIDE_diagnosis_skMI_foo, 1)
        Pearson_fit_mean = np.mean(ABIDE_diagnosis_Pearson_foo, 1)
        Pearson_fit_std = np.std(ABIDE_diagnosis_Pearson_foo, 1)

        _plt.plot(num_attr, MI_fit_mean, label=dep_measure, color="b")
        _plt.fill_between(num_attr,
                          (MI_fit_mean + MI_fit_std * norm.ppf(0.025)),
                          (MI_fit_mean + MI_fit_std * norm.ppf(0.975)),
                          color="b",
                          alpha=.1)

        _plt.plot(num_attr,
                  skMI_fit_mean,
                  label="Mutual Information by skLearn",
                  color="y")
        _plt.fill_between(num_attr,
                          (skMI_fit_mean + skMI_fit_std * norm.ppf(0.025)),
                          (skMI_fit_mean + skMI_fit_std * norm.ppf(0.975)),
                          color="y",
                          alpha=.1)

        _plt.plot(num_attr,
                  Pearson_fit_mean,
                  label="Pearson Correlation",
                  color="g")
        _plt.fill_between(
            num_attr, (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.025)),
            (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.975)),
            color="g",
            alpha=.1)
        _plt.title(fun_name)
        _plt.legend()


dep_measure_list = []
for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]

for dep_measure in dep_measure_list:
```

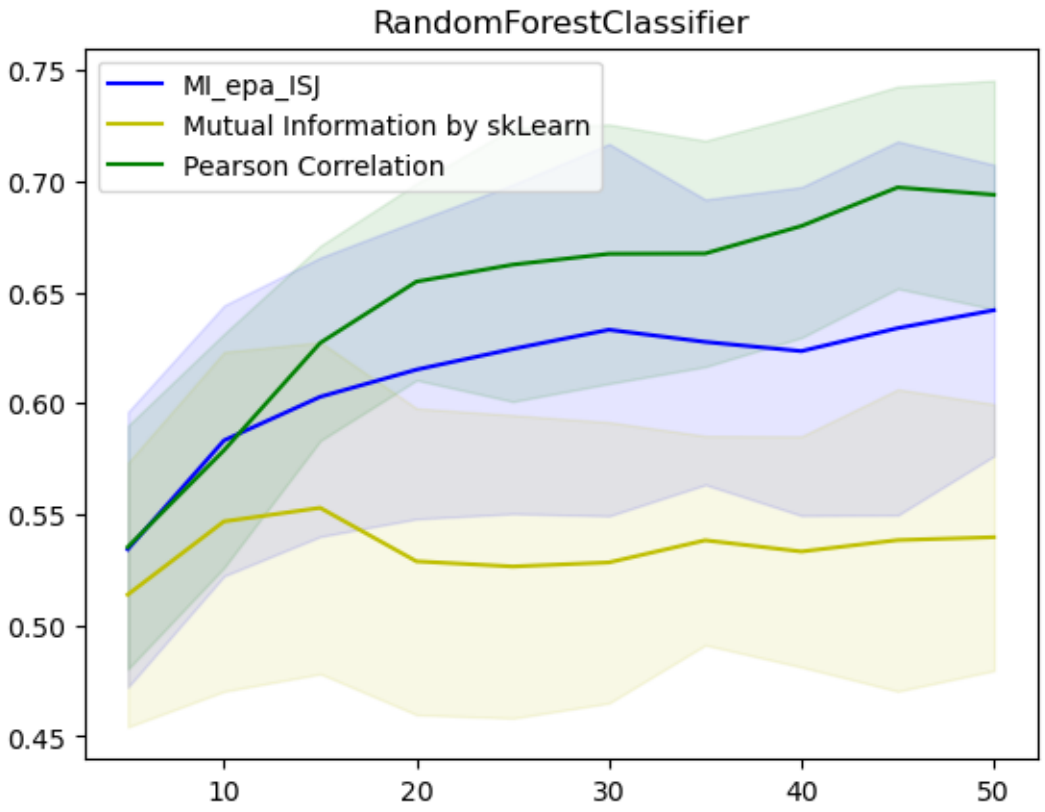
```
    for fun_name in [
            "MLPClassifier", "LogisticRegressionCV_l2",
            "LogisticRegressionCV_l1", "LogisticRegressionCV_ElasticNet",
            "RandomForestClassifier", "LogisticRegression"
    ]:
        if dep_measure == "MI_epa_ISJ":
            plot_results(plt, fun_name, dep_measure=dep_measure)
            plt.savefig(r"./ABIDE_predict_diagnosis/" + fun_name + dep_measure)
            plt.show()
```




LogisticRegressionCV_l2
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.8
0.7
0.6
0.5
0.4
10
20
30
40
50


LogisticRegressionCV_l1
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
10
20
30
40
50


LogisticRegressionCV_ElasticNet
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.8
0.7
0.6
0.5
0.4
10
20
30
40
50

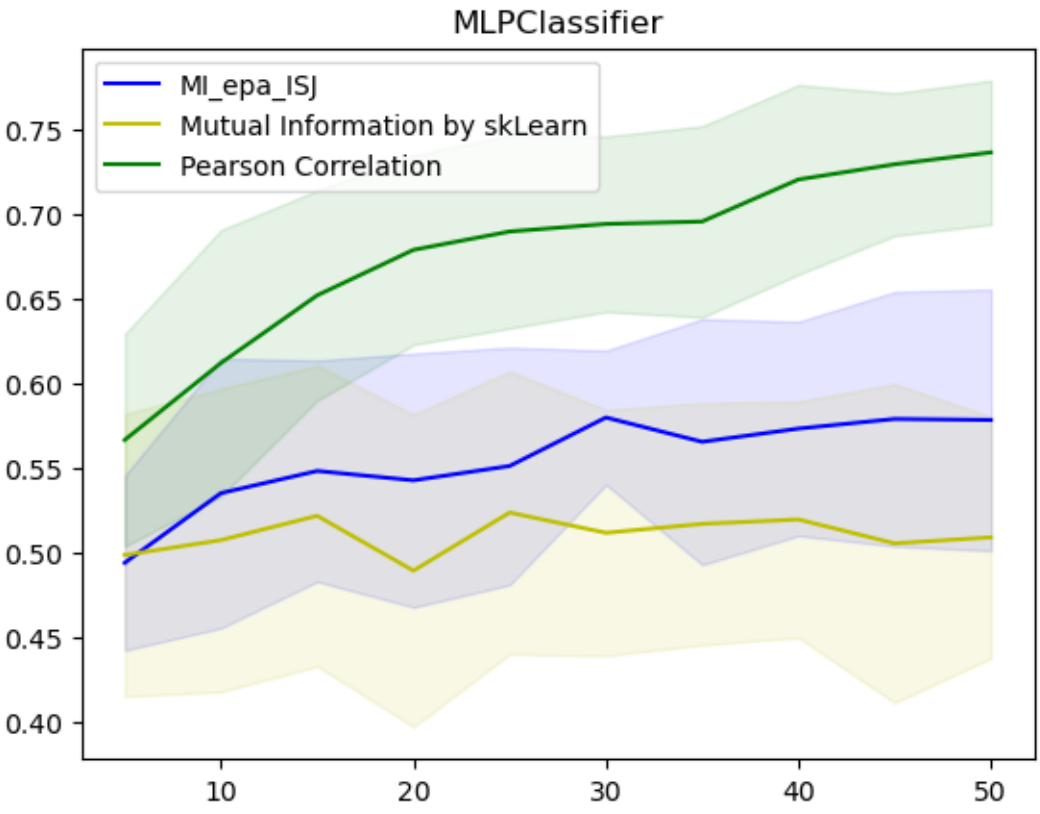


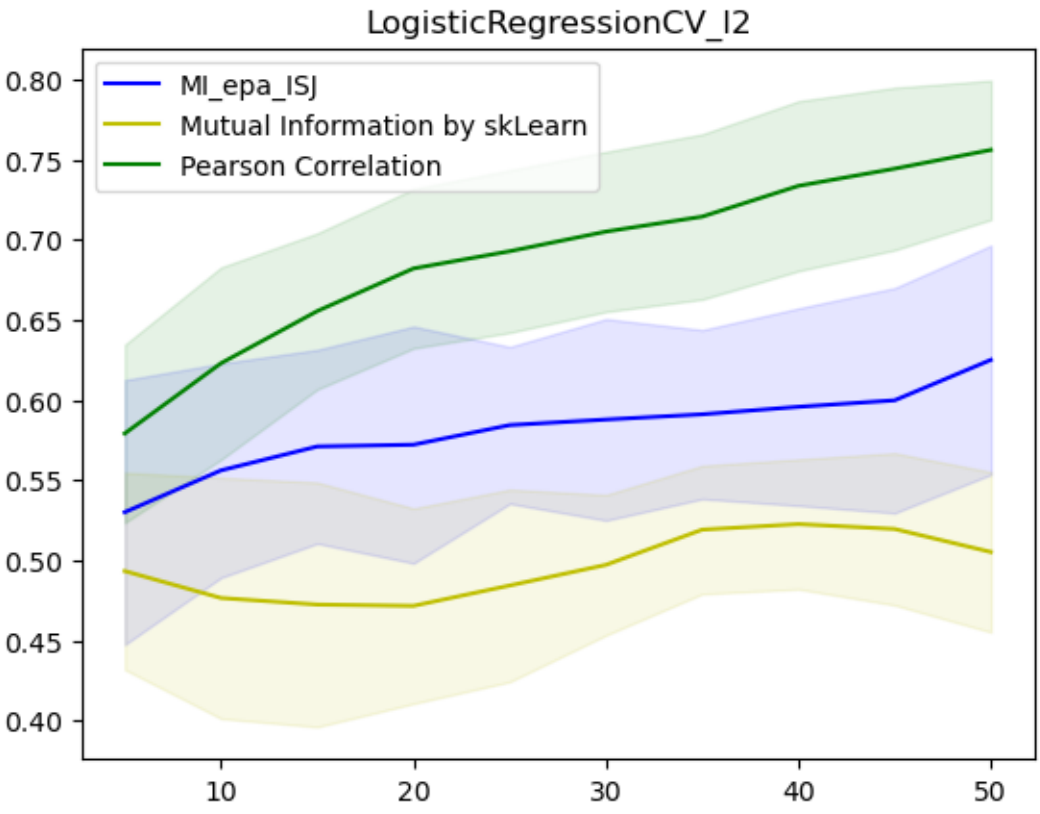
<Figure size 640x480 with 0 Axes>

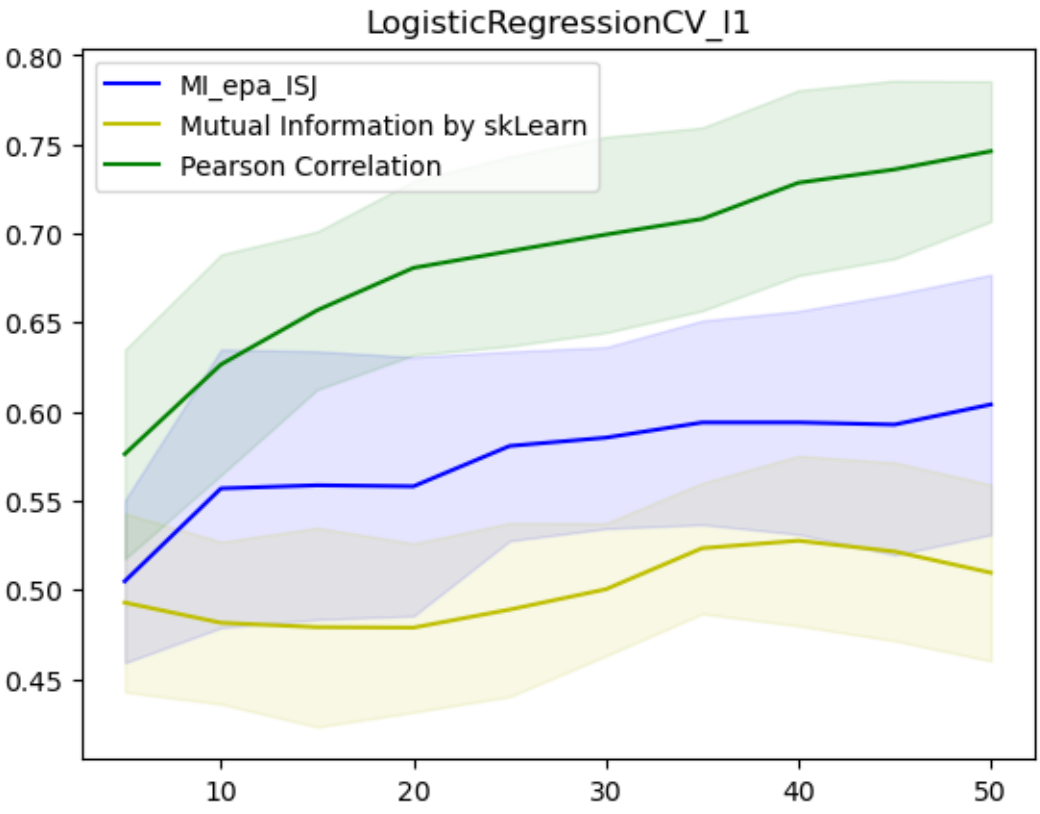
[18]:
```
import os


def plot_results(_plt, fun_name, dep_measure):
    if os.path.isfile(
            r"./ABIDE_poly3_predict_diagnosis/
 ↪ABIDE_poly3_diagnosis_{dep_measure}_{fun_name}.npy"
            .format(fun_name=fun_name, dep_measure=dep_measure)
    ) and os.path.isfile(
            r"./ABIDE_poly3_predict_diagnosis/
 ↪ABIDE_poly3_diagnosis_skMI_{fun_name}.npy"
            .format(fun_name=fun_name)
    ) and os.path.isfile(
            r"./ABIDE_poly3_predict_diagnosis/
 ↪ABIDE_poly3_diagnosis_Pearson_{fun_name}.npy"
            .format(fun_name=fun_name)):
        columns = np.load(r"./ABIDE_columns.npy")
        ABIDE_diagnosis_MI_foo = np.load(
```

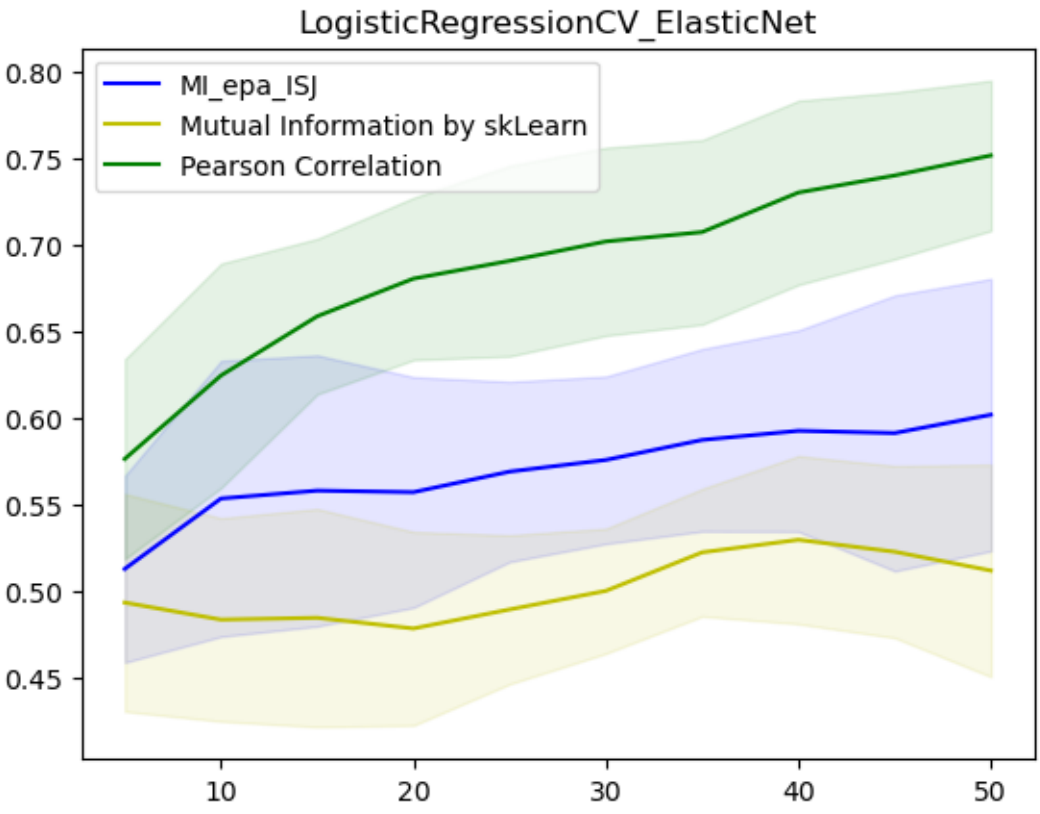
```
            r"./ABIDE_poly3_predict_diagnosis/
↪ABIDE_poly3_diagnosis_{dep_measure}_{fun_name}.npy"
            .format(fun_name=fun_name, dep_measure=dep_measure))
        ABIDE_diagnosis_skMI_foo = np.load(
            r"./ABIDE_poly3_predict_diagnosis/
↪ABIDE_poly3_diagnosis_skMI_{fun_name}.npy"
            .format(fun_name=fun_name))
        ABIDE_diagnosis_Pearson_foo = np.load(
            r"./ABIDE_poly3_predict_diagnosis/
↪ABIDE_poly3_diagnosis_Pearson_{fun_name}.npy"
            .format(fun_name=fun_name))
        num_attr = list(
            map(int,
                np.around(np.linspace(
                    0, 50, 10 +
                    1)[1:]).tolist()))  # ADJUST this based on actual settings

        MI_fit_mean = np.mean(ABIDE_diagnosis_MI_foo, 1)
        MI_fit_std = np.std(ABIDE_diagnosis_MI_foo, 1)
        skMI_fit_mean = np.mean(ABIDE_diagnosis_skMI_foo, 1)
        skMI_fit_std = np.std(ABIDE_diagnosis_skMI_foo, 1)
        Pearson_fit_mean = np.mean(ABIDE_diagnosis_Pearson_foo, 1)
        Pearson_fit_std = np.std(ABIDE_diagnosis_Pearson_foo, 1)

        _plt.plot(num_attr, MI_fit_mean, label=dep_measure, color="b")
        _plt.fill_between(num_attr,
                          (MI_fit_mean + MI_fit_std * norm.ppf(0.025)),
                          (MI_fit_mean + MI_fit_std * norm.ppf(0.975)),
                          color="b",
                          alpha=.1)

        _plt.plot(num_attr,
                  skMI_fit_mean,
                  label="Mutual Information by skLearn",
                  color="y")
        _plt.fill_between(num_attr,
                          (skMI_fit_mean + skMI_fit_std * norm.ppf(0.025)),
                          (skMI_fit_mean + skMI_fit_std * norm.ppf(0.975)),
                          color="y",
                          alpha=.1)

        _plt.plot(num_attr,
                  Pearson_fit_mean,
                  label="Pearson Correlation",
                  color="g")
        _plt.fill_between(
            num_attr, (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.025)),
```

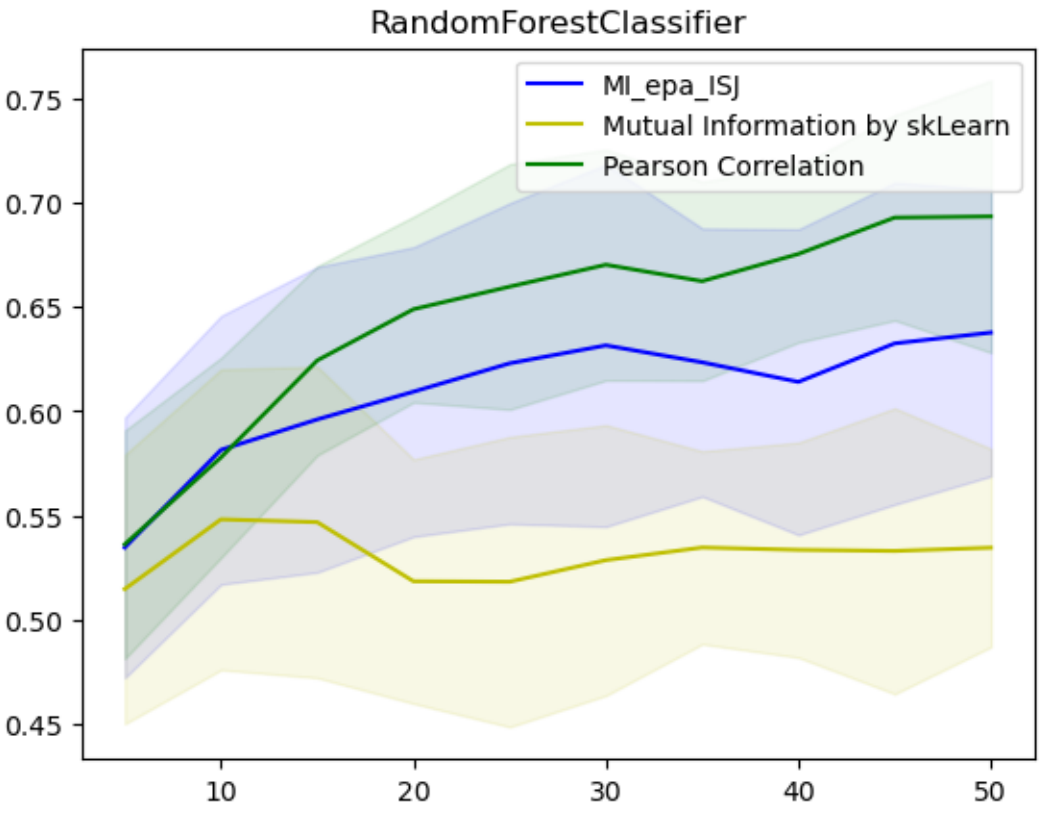
```
            (Pearson_fit_mean + Pearson_fit_std * norm.ppf(0.975)),
            color="g",
            alpha=.1)
        _plt.title(fun_name)
        _plt.legend()


dep_measure_list = []
for _kernel in [
        'gaussian', 'exponential', 'box', 'tri', 'epa', 'biweight',
        'triweight', 'tricube', 'cosine'
]:
    for _bw in ['silverman', 'scott', 'ISJ']:
        dep_measure_list += ["MI_{kernel}_{bw}".format(kernel=_kernel, bw=_bw)]

for dep_measure in dep_measure_list:
    for fun_name in [
            "MLPClassifier", "LogisticRegressionCV_l2",
            "LogisticRegressionCV_l1", "LogisticRegressionCV_ElasticNet",
            "RandomForestClassifier", "LogisticRegression"
    ]:
        if dep_measure == "MI_epa_ISJ":
            plot_results(plt, fun_name, dep_measure=dep_measure)
            plt.savefig(r"./ABIDE_poly3_predict_diagnosis/" + fun_name +
                        dep_measure)
            plt.show()
```


MLPClassifier
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
10
20
30
40
50


LogisticRegressionCV_l2
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
10
20
30
40
50


LogisticRegressionCV_l1
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
10
20
30
40
50


LogisticRegressionCV_ElasticNet
MI_epa_ISJ
Mutual Information by skLearn
Pearson Correlation
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
10
20
30
40
50




```
<Figure size 640x480 with 0 Axes>
```

[ ]: