Junifer and Julearn: From Neuroimaging to Machine Learning models without expert-level coding skills

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Introduction

- Current increasing popularity in Neuroimaging + Machine Learning [1] due to big data and computing power.
- But…
  - High impact on results from decisions
    - in data processing [2]
    - In ML modelling [3]
  - Misconceptions in ML lead to distorted or even invalid findings [4]
  - Early-career researchers require
    - Domain-specific knowledge (e.g. behavioral sciences, biology)
    - ML-specific knowledge (e.g. cross-validation, learning algorithms)
    - Highly developed technical skills (e.g. High-Performance Computing)

Goals

Develop tools:

- Minimal coding
  - If possible, no coding at all
- Easy to learn, use and share
  - But still powerful, including complex methods!
- Suitable for users from diverse backgrounds
  - even with non-STEM formal training
- Minimize user-related errors, E.g.:
  - Wrong template spaces in neuroimaging
  - Data-leakage in ML [4]
- Extensible libraries (e.g. allow to develop novel methods)

Neuroimaging Feature Extraction

- Pipeline Configuration Tool

- No-code tool (YAML file)
- Easy to run for entire datasets
  - HPC or local (GNU-Parallels)
- Built on state-of-the-art tools: AFNI, FSL, ANTS, Nilearn
- Examples:

https://juaml.github.io/junifer

```yaml
workdir: /tmp

datagrabber:
    kind: DataladAOMICID1000
    native_t1w: true

preprocess:
  - kind: fMRIPrepConfoundRemover
    detrend: true
    standardize: true
    strategy:
        motion: full
        wm_csf: full
        global_signal: full
    low_pass: 0.08
    high_pass: 0.01
    masks:
      - inherit
      - compute_epi_mask
      - threshold: 0
  - kind: SpaceWarper
    reference: T1w
    on: BOLD
    using: ants

markers:
  - name: FC-Schaefer100x17
    kind: FunctionalConnectivityParcels
    cor_method: correlation
    parcellation: Schaefer100x17
    masks:
      - inherit

storage:
  kind: HDF5FeatureStorage
  uri: /data/group/riseml/fraimondo/2024_HIP/features/ds003097_FC_native/ds003097_FC_native.hdf5

queue:
  jobname: aomic_fc_native
  kind: HTCondor
  env:
    kind: conda
    name: neurodc
  mem: 8G
  disk: 5G
  verbose: info
```

Dataset to use (can also be specified in terms of file-naming patterns)

One or more data transformation steps

Remove Confounds (e.g. motion parameters)

Warp-back to native space using ANTS

One or more markers

Compute functional connectivity

Storage specification

Run in HPC:

- 1 job per subject using a HTCondor queue
- Use a conda environment
- Ask for 8G of RAM and 5G of disk per job

```yaml
workdir: /tmp

datagrabber:
  kind: DataladAOMICID1000
  types:
    - FreeSurfer

markers:
  - name: brainprint
    kind: BrainPrint

storage:
  kind: HDF5FeatureStorage
  uri: ./storage/brainprint/aomicid1000_brainprint.hdf5
```

ShapeDNA [5] (BrainPrint [6]) in 14 lines!

Machine Learning

- Easily create and evaluate models
  - Tabular data, using pandas
- Estimate model performance using cross-validation
  - Prevent data-leakage
- Easy hyperparameter tuning (using nested CV)
- Built on top of scikit-learn [7]
- Example:

https://juaml.github.io/julearn

```python
from junifer.storage import HDF5FeatureStorage
from julearn.api import run_cross_validation
from julearn.pipeline import PipelineCreator
import pandas as pd
import seaborn as sns
from pathlib import Path

t_path = Path(__file__).parent

storage = HDF5FeatureStorage(t_path / "data/aomicid1000_brainprint.hdf5")

df_eigen = storage.read_df("FreeSurfer_brainprint_eigenvalues")
df_areas = storage.read_df("FreeSurfer_brainprint_areas")
df_volumes = storage.read_df("FreeSurfer_brainprint_volumes")
df_volumes = df_volumes.reset_index().set_index("subject")
df_volumes["gm_vol"] = df_volumes["lh-pial-2d"] + df_volumes["rh-pial-2d"]

df_demographics = pd.read_csv(t_path / "data/participants.tsv", sep="\t")
df_demographics.rename(columns={"participant_id": "subject"}, inplace=True)
df_demographics = df_demographics.set_index("subject")

columns = [
    "4th-Ventricle", "Brain-Stem", "Left-Cerebellum-White-Matter",
    "Left-Cerebellum-Cortex", "Left-Thalamus-Proper", "Left-Caudate",
    "Left-Putamen", "Left-Pallidum", "Left-Hippocampus", "Left-Amygdala",
    "Left-Accumbens-area", "Left-VentralDC", "Right-Cerebellum-White-Matter",
    "Right-Cerebellum-Cortex", "Right-Thalamus-Proper", "Right-Caudate",
    "Right-Putamen", "Right-Pallidum", "Right-Hippocampus", "Right-Amygdala",
    "Right-Accumbens-area", "Right-VentralDC", "lh-white-2d", "rh-white-2d",
    "lh-pial-2d","rh-pial-2d",
]

df_data = df_eigen[columns].unstack(-1).reset_index().set_index("subject")
df_data.columns = df_data.columns.map(
    lambda x: x if isinstance(x, str) else f"{x[0]}_{x[1]}"
)
df_data = df_data.join(df_demographics)
df_data = df_data.join(df_volumes["gm_vol"])


X = [x for x in df_data.columns if any(x.startswith(y) for y in columns)]
X_types = {"continuous": [".*"]}

creator = PipelineCreator(problem_type="classification")
creator.add("zscore")
creator.add(
    "svm",
    C=(0.001, 100, "log-uniform"),
)

search_params = {
    "kind": "optuna",
    "cv": 5,
}
scores, model, inspector = run_cross_validation(
    X=X,
    y="sex",
    data=df_data,
    X_types=X_types,
    search_params=search_params,
    model=creator,
    return_train_score=True,
    return_inspector=True,
    cv=5,
)

predictions = inspector.folds.predict()
to_merge = df_data[["sex", "gm_vol"]].iloc[predictions.index]
predictions.index = to_merge.index
to_plot = pd.concat([predictions, to_merge], axis=1)

to_plot["correct"] = to_plot["repeat0_p0"] == to_plot["target"]
sns.boxplot(data=to_plot, x="sex", hue="correct", y="gm_vol")
```

Read data from Junifer (or other tabular format)

Rename columns and combine DataFrames

Define features and feature types

Easy model-specification (e.g. SVM):

- Tune the optimal C from a log-uniform distribution [0.001, 100]

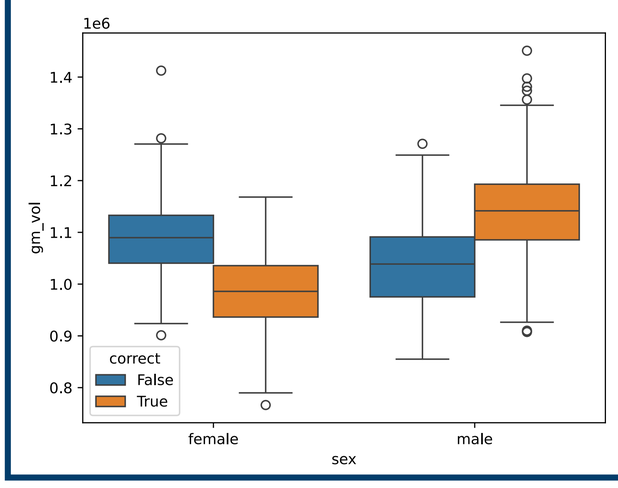
Use Optuna for hyperparameter tuning

Evaluate the model using Cross-Validation

Inspect the results:

- E.g. do we have a bias?

Conclusion



- Building and evaluating ML models from neuroimaging is not an easy task.
  - Even reproducing them is hard! [8]
- Interpreting results to obtain insights can be tricky [9]
  - E.g. sex prediction is biased by the total intracranial volume
- Junifer and Julearn enable domain experts without highly-developed programming and technical skills to analyze brain images and build complex ML pipelines
- Neuroimaging and ML experts can easily extend the libraries with custom methods.
- We can't showcase all the features here (e.g.)
  - Neuroimaging-specific models:
    - Connectome-based Predictive Modelling [10]
  - Interactive ML model comparison plots
    - With corrected t-tests for ML [11]
  - Easily share features and code
- Core developers from the Applied Machine Group, at the Institute of Neuroscience and Medicine – 7: Brain and Behavior, at Jülich Research Center: We can understand ML and brain-imaging research questions.

TRY IT YOURSELF!

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