

# NeuroCAPs: A Python Package for Performing Co-Activation Patterns Analyses on Resting-State and Task-Based fMRI Data

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DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

## Software

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Submitted: 01 January 1970

Published: unpublished

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## Summary

Co-Activation Patterns (CAPs) is a dynamic functional connectivity technique that clusters similar spatial distributions of brain activity. NeuroCAPs is an open-source Python package that makes CAPs analysis accessible to neuroimaging researchers for preprocessed resting-state or task-based fMRI data. The package is optimized for fMRIPrep-preprocessed data ([Esteban et al., 2019](#)), leveraging fMRIPrep's robust, BIDS-compliant outputs.

## Background

Numerous fMRI studies employ static functional connectivity (sFC) techniques to analyze correlative activity within and between brain regions. However, these approaches assume functional connectivity patterns, which change within seconds ([Jiang et al., 2022](#)), remain stationary throughout the entire data acquisition period ([Hutchison et al., 2013](#)).

Unlike sFC approaches, dynamic functional connectivity (dFC) methods enable the analysis of dynamic functional states, which are characterized by consistent, replicable, and distinct periods of time-varying brain connectivity patterns ([Rabany et al., 2019](#)). Among these techniques, CAPs analysis aggregates similar spatial distributions of brain activity using a clustering algorithm (i.e., k-means) to capture the dynamic nature of brain activity ([Liu et al., 2013, 2018](#)).

## Statement of Need

The CAPs workflow can be programmatically time-consuming as researchers must:

1. apply spatial dimensionality reduction to timeseries data
2. perform nuisance regression and remove high-motion volumes
3. concatenate timeseries data from multiple subjects into a single matrix
4. implement k-means clustering with optimal cluster selection
5. generate visualizations for CAP interpretation

While excellent CAPs toolboxes exist, they are often implemented in proprietary languages such as MATLAB (TbCAPs ([Bolton et al., 2020](#))), lack comprehensive end-to-end analytical pipelines for both resting-state and task-based fMRI data with temporal dynamic metrics and visualization capabilities (capcalc ([Frederick & Drucker, 2022](#))), or are comprehensive, but generalized toolboxes for evaluating and comparing different dFC methods (pydFC ([Torabi et al., 2024](#))).

NeuroCAPs provides an accessible Python package for end-to-end CAPs analysis, spanning

fMRI post-processing through computation of temporal metrics and creation of visualizations. However, many of NeuroCAPs' post-processing functionalities assumes that fMRI data is organized in a BIDS compliant directory (Yarkoni et al., 2019) and is optimized for fMRIPrep (Esteban et al., 2019) or fMRIPrep-like pipelines such as NiBabies (Goncalves et al., 2025). Furthermore, NeuroCAPs is limited to the k-means algorithm for clustering, a choice that aligns with the original CAPs methodology (Liu et al., 2013) and its prevalence in the CAPs literature.

## Modules

The core functionalities of NeuroCAPs are concentrated in three modules:

1. neurocaps.extraction contains the TimeseriesExtractor class, which:
  - leverages Nilearn's (contributors, n.d.) NiftiLabelsMasker for denoising and spatial dimensionality reduction using deterministic parcellations (e.g., Schaefer (Schaefer et al., 2018), AAL (Tzourio-Mazoyer et al., 2002), etc)
  - removes high-motion volumes using fMRIPrep-derived framewise displacement (FD) values
  - reports quality control metrics for motion and non-steady state volumes
2. neurocaps.analysis contains the CAP class for performing the CAPs analysis, as well as standalone functions.
  - The CAP class:
    - identifies CAPs via k-means clustering (Pedregosa et al., 2011) with optimized cluster selection (e.g., silhouette, elbow (Arvai, 2023), etc)
    - computes subject-level temporal metrics (e.g., temporal fraction, transition probabilities, etc)
    - converts CAPs to NIFTI statistical maps
    - integrates multiple plotting libraries (Gale et al., 2021; Hunter, 2007; Inc., n.d.; Waskom, 2021) for diverse visualizations
  - Standalone functions: provides tools for within-run ROI standardization (Harris et al., 2020), merging timeseries across sessions/tasks and creating group-averaged transition matrices.
3. neurocaps.utils contains utility functions for:
  - fetching non-default (i.e., Schaefer and AAL) preset parcellation approaches (i.e., 4S, HCPex (Huang et al., 2022), and Gordon (Gordon et al., 2016))
  - generating custom parcellation approaches from tabular metadata
  - customizing plots and simulating data

## Workflow

The following code demonstrates basic usage of NeuroCAPs (with simulated data) to perform CAPs analysis, [a version using real data is also available](#).

1. Extract timeseries data

```
import numpy as np
from neurocaps.extraction import TimeseriesExtractor
from neurocaps.utils import simulate_bids_dataset

# Set seed
np.random.seed(0)
```

```
# Generate a BIDS directory with fMRIPrep derivatives
bids_root = simulate_bids_dataset(n_subs=3, n_runs=1, n_volumes=100, task_name="rest")

# Set the parcel approach
parcel_approach = {"Schaefer": {"n_rois": 100, "yeo_networks": 7}}

# List of fMRIPrep-derived confounds for nuisance regression
acompcor_names = [f"a_comp_cor_0{i}" for i in range(5)]
confound_names = ["cosine*", "trans*", "rot*", *acompcor_names]

# Initialize extractor with signal cleaning parameters
extractor = TimeseriesExtractor(
    space="MNI152NLin2009cAsym",
    parcel_approach=parcel_approach,
    confound_names=confound_names,
    standardize=False,
    # Run discarded if >30% of volumes exceed FD threshold
    fd_threshold={"threshold": 0.90, "outlier_percentage": 0.30},
)

# Extract timeseries
extractor.get_bold(bids_dir=bids_root, task="rest", tr=2, n_cores=1, verbose=False)

# Check QC information
qc_df = extractor.report_qc()
print(qc_df)
```

Subject_ID	Run	Mean_FD	Std_FD	Frames_Scrubbed	Frames_Interpolated	Mean_High_Motion_Length	Std_High_Motion_Length	N_Dummy_Scans
0	0 run-0	0.516349	0.289657	9	0	1.125000	0.330719	NaN
1	1 run-0	0.526343	0.297550	17	0	1.133333	0.339935	NaN
2	2 run-0	0.518041	0.273964	8	0	1.000000	0.000000	NaN

Figure 1: Quality Control Dataframe.

2. Use k-means clustering to identify the optimal number of CAPs from the data using a heuristic

```
from neurocaps.analysis import CAP
from neurocaps.utils import PlotDefaults

cap_analysis = CAP(parcel_approach=extractor.parcel_approach, groups=None)

plot_kwargs = {**PlotDefaults.get_caps(), "figsize": (4, 3), "step": 2}

# Find optimal CAPs (2-20) using silhouette method; results are stored
cap_analysis.get_caps(
    subject_timeseries=extractor.subject_timeseries,
    n_clusters=range(2, 21),
    standardize=True,
    cluster_selection_method="silhouette",
    max_iter=500,
    n_init=10,
    show_figs=True,
    **plot_kwargs,
)
```

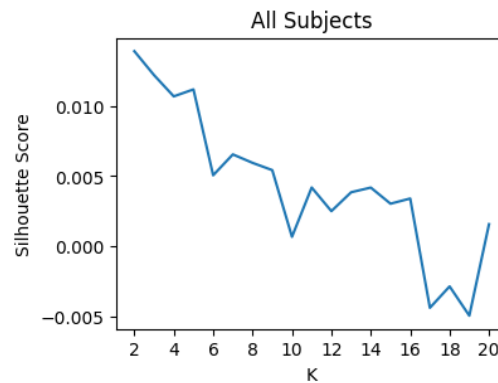


Figure 2: Silhouette Score Plot.

77 3. Compute temporal dynamic metrics for downstream statistical analyses

```
metric_dict = cap_analysis.calculate_metrics(
    extractor.subject_timeseries, metrics=["temporal_fraction"]
)
print(metric_dict["temporal_fraction"])
```

	Subject_ID	Group	Run	CAP-1	CAP-2
0	0	All Subjects	run-0	0.505495	0.494505
1	1	All Subjects	run-0	0.530120	0.469880
2	2	All Subjects	run-0	0.521739	0.478261

Figure 3: Temporal Fraction Dataframe.

78 Note that CAP-1 is the dominant brain state across subjects (highest frequency).

79 4. Visualize CAPs

```
surface_kwargs = {**PlotDefaults.caps2surf(), "layout": "row", "size": (500, 100)}

radar_kwargs = {**PlotDefaults.caps2radar(), "height": 400, "width": 485}
radar_kwargs["radialaxis"] = {"range": [0, 0.4], "tickvals": [0.1, "", "", 0.4]}
radar_kwargs["legend"] = {"yanchor": "top", "y": 0.75, "x": 1.15}

cap_analysis.caps2surf(**surface_kwargs).caps2radar(**radar_kwargs)
```

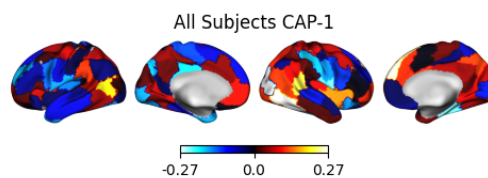


Figure 4: CAP-1 Surface Image.

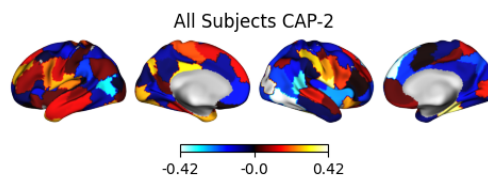


Figure 5: CAP-2 Surface Image.

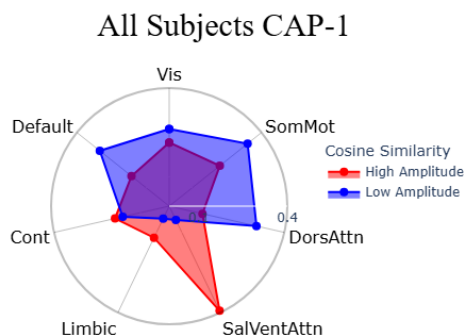


Figure 6: CAP-1 Radar Image.

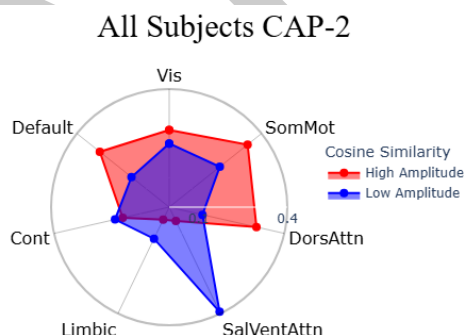


Figure 7: CAP-2 Radar Image.

Radar plots show network alignment (measured by cosine similarity): “High Amplitude” represents alignment to activations ( $> 0$ ), “Low Amplitude” represents alignment to deactivations ( $< 0$ ).

Each CAP can be characterized using either maximum alignment (CAP-1: Vis+/SomMot-; CAP-2: SomMot+/Vis-) or predominant alignment (“High Amplitude” – “Low Amplitude”; CAP-1: SalVentAttn+/SomMot-; CAP-2: SomMot+/SalVentAttn-).

```
import pandas as pd
```

```
for cap_name in cap_analysis.caps["All Subjects"]:
    df = pd.DataFrame(cap_analysis.cosine_similarity["All Subjects"][cap_name])
    df["Net"] = df["High Amplitude"] - df["Low Amplitude"]
    df["Regions"] = cap_analysis.cosine_similarity["All Subjects"]["Regions"]
    print(df, "\n")
```

	High Amplitude	Low Amplitude	Net	Regions
0	0.220327	0.199130	0.021197	Vis
1	0.244341	0.154648	0.089693	SomMot
2	0.141356	0.399899	-0.258543	DorsAttn
3	0.300487	0.103134	0.197352	SalVentAttn
4	0.104964	0.092692	0.012272	Limbic
5	0.194957	0.160273	0.034684	Cont
6	0.263373	0.308228	-0.044855	Default

Figure 8: CAP-1 Network Alignment Dataframe.

	High Amplitude	Low Amplitude	Net	Regions
0	0.199130	0.220327	-0.021197	Vis
1	0.154648	0.244341	-0.089693	SomMot
2	0.399899	0.141356	0.258543	DorsAttn
3	0.103134	0.300487	-0.197352	SalVentAttn
4	0.092692	0.104964	-0.012272	Limbic
5	0.160273	0.194957	-0.034684	Cont
6	0.308228	0.263373	0.044855	Default

Figure 9: CAP-2 Network Alignment Dataframe.

## Documentation

Comprehensive documentation and tutorials can be found at <https://neurocaps.readthedocs.io/> and <https://github.com/donishadsmith/neurocaps>.

## Acknowledgements

Funding from the Dissertation Year Fellowship Program at Florida International University supported NeuroCAPs' refinement and expansion.

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