QPPLab: A generally applicable software package for detecting, analyzing, and visualizing large-scale quasiperiodic spatiotemporal patterns (QPPs) of brain activity

Nan Xu[1], Behnaz Yousefi[1], Nmachi Anumba[1], Theodore J. LaGrow[3], Xiaodi Zhang[1], Shella Keilholz[1]

[1]Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, GA, United States
[3]Electrical and Computer Engineering, Georgia Tech, Atlanta, GA, United States

Abstract

One prominent brain dynamic process detected in functional neuroimaging data is large-scale quasi-periodic patterns (QPPs) which display spatiotemporal propagations along brain cortical gradients. QPP associates with the infraslow neural activity related to attention and arousal fluctuations and has been identified in both resting and task-evoked brains across various species. Several QPP detection and analysis tools were developed for distinct applications with study-specific parameter methods. This MATLAB package provides a simplified and user-friendly generally applicable toolbox for detecting, analyzing, and visualizing QPPs from fMRI timeseries of the brain. This paper describes the software functions and presents its ease of use on any brain datasets.

Keywords

Infraslow activity, quasiperiodic patterns, spatiotemporal brain dynamics, functional MRI

Metadata

Nr	Code metadata description	
C1	Current code version	v1
C2	Permanent link to code/repository used for this code version	https://github.com/GT-EmoryMINDlab/QPPLab
C3	Permanent link to reproducible capsule	N/A
C4	Legal code license	MIT License
C5	Code versioning system used	git
C6	Software code languages, tools and services used	MATLAB
C7	Compilation requirements, operating environments and dependencies	MATLAB R2018 or a later version
C8	If available, link to developer documentation/manual	https://github.com/GT-EmoryMINDlab/QPPLab/blob/main/README.md
C9	Corresponding author	im.nan.xu@gmail.com

1. Motivation and significance

The infraslow BOLD fluctuations in the brain have been the subject of much research, revealing new insights into the brain's functional architecture and how it changes during tasks, development, and disease (Fox & Raichle, 2007). One particular type of spatiotemporal dynamic processes that has emerged from this research is the quasi-periodic pattern (QPP), which consists of a reproducible pattern of spatiotemporal evolution of activity that reoccurs over time. QPPs exhibit an alternation of high and low activity in widespread brain areas with the propagation of activity along the cortex, which have been widely observed in resting and task-evoked rodents (Belloy, Naeyaert, et al., 2018; Belloy, Shah, et al., 2018; Majeed et al., 2011;

Thompson et al., 2014; Xu, Smith, et al., 2023) as well as in human brains (Bolt et al., 2022; Majeed et al., 2011; Raut et al., 2021; Xu, Zhang, et al., 2023; Yousefi & Keilholz, 2021).

Multiple QPPs have been recognized as capturing intrinsic activity dynamics (Bolt et al., 2022; Yousefi & Keilholz, 2021). The primary (or the strongest) QPP (referred to here as QPP1) shows prominent anticorrelation between the default mode network (DMN) and task-positive network (TPN) across species (Belloy, Naeyaert, et al., 2018; Majeed et al., 2011; Raut et al., 2021; Yousefi et al., 2018; Yousefi & Keilholz, 2021) when global signal regression has been applied. QPP1 is shown to correlate with infraslow neural activity (Grooms et al., 2017; Thompson et al., 2014), and is found to be affected by sustained attention, working memory tasks (Abbas, Bassil, et al., 2019; Abbas, Belloy, et al., 2019), and arousal fluctuations (Raut et al., 2021).

An initial detection algorithm for QPP1 was developed by (Majeed et al., 2011) to analyze fMRI data collected from brain voxels. This algorithm employs correlation-based and iterative techniques to identify similar segments within functional timecourses. These segments are then averaged to create a representative spatiotemporal template. This algorithm has been popularly used in both rodent and human studies (Belloy, Naeyaert, et al., 2018; Belloy, Shah, et al., 2018; Majeed et al., 2011). Subsequent efforts adapted this algorithm for fMRI data extracted from the Brainnetome atlas (Abbas, Belloy, et al., 2019) or from the Glasser atlas (Yousefi et al., 2018; Yousefi & Keilholz, 2021), enabling the observation of region of interest (ROI) and network-based QPPs throughout the entire human brain.

More recently, an enhanced version of the QPP detection algorithm was introduced by (Yousefi & Keilholz, 2021). This advanced algorithm identified not only QPP1 but also additional QPPs such as the QPP2 and QPP3 in humans. The algorithm involved regressing QPP1 from the original functional data, resulting in the detection of QPP2 by using the same iterative approach on the residuals. These supplementary QPPs were found to involve coordinated propagation of activity along functional gradients across the entire brain, contributing to functional brain connectivity.

Despite the thorough identification and analysis of QPPs in multiple species, existing software tools are constrained by their strong dependence on study-specific settings, such as specific atlas schemes (Abbas, Belloy, et al., 2019; Yousefi & Keilholz, 2021), certain brain regions (Majeed et al., 2011), particular species (Belloy, Naeyaert, et al., 2018), or an exclusive emphasis on QPP1s (e.g., Abbas, Belloy, et al., 2019; Yousefi et al., 2018), etc. This reliance not only made the tools less versatile but also required users to redundantly specify multiple parameters at various stages, leading to a complex and error-prone process. There has been a persistent need for a user-friendly software package that could offer a parameter-simplified and universally applicable solution. To address this need, we present "*QPPLab*". This open-source MATLAB package for QPP detection, analysis, and visualization incorporates several esteemed algorithms and analytical methods. In *QPPLab*, users simply set a select few global parameters at the beginning. The software then skillfully deduces and establishes the related parameters via internal functions, mitigating redundancy and potential inconsistencies. By minimizing the need for manual, study-specific parameter adjustments, *QPPLab* stands out as a software

package designed to provide researchers with a more streamlined, consistent, and universally applicable tool for QPP analysis across various datasets (Xu, Smith, et al., 2023; Xu, Zhang, et al., 2023; Seeburger et al, 2023).

2.   Software description

QPPLab was modified and expanded based on the latest QPP analytic tools (Yousefi & Keilholz, 2021), which can detect, analyse, and visualize QPP1 as well as additional QPPs from functional neuroimaging timeseries of the brain. This software also encompasses analytical and visualization techniques introduced in (Abbas, Belloy, et al., 2019; Majeed et al., 2011; Xu, Smith, et al., 2023; Yousefi et al., 2018; Yousefi & Keilholz, 2021).

The main QPP detection algorithm (Majeed et al., 2011) and its two major outputs are described in Fig. 1. In brief, a 4-step procedure was performed: 1) an initial segment with a fixed window length is selected at a random starting point from the functional timecourse; 2) this selected segment is correlated with a segment with the same window length that is sliding from the beginning to the end of the timecourse at every timepoint, which results in a timecourse of sliding correlation values; 3) the segments, that are corresponding to the local maxima of the correlation timecourse, are then averaged to obtain the new segment; 4) steps 2-3 are iterated until the averaged segment and the selected segment converge.

Figure 1   QPP detection algorithm and its output format (adapted from Yousefi & Keilholz, 2021, Fig. S2). The output of QPP includes a) a final template of QPP and b) a correlation timecourse of the final template.

Based on the approach introduced in (Yousefi & Keilholz, 2021), *QPPLab* includes an extended version of this detection algorithm. Specifically, multiple initial segments are selected, and the 4-step procedure is performed for each selection. The averaged QPP with the greatest summation of local maxima of sliding correlations will be selected as the final template.

QPPLab offers two distinct modes of operation: a fast detection option and a robust detection option. The rapid mode involves the random selection of a subset of initial segments from the timecourse (e.g., Majeed et al., 2011; Yousefi et al., 2018), while the robust mode comprehensively considers all potential initial segments present in the timecourse (e.g., Yousefi & Keilholz, 2021; Xu, Smith, et al., 2023). This two-mode operation facilitates flexibility in tailoring the analysis according to the research needs. In addition, *QPPLab* extends the functionality to accommodate the specification of undesirable timepoints within the fMRI scan data. By systematically excluding these problematic timepoints from the algorithmic process, the

resultant QPP outcomes can effectively eliminate the confounding of motion-induced distortions and other potential artifacts.

Notably, *QPPLab* utilizes an algorithm based on correlation and regressions, and can identify multiple spatiotemporal patterns. These spatiotemporal are analogous to the spatiotemporal patterns delineated by a sophisticated principal component analysis approach (Bolt et al., 2022). For instance, in the absence of the application of global signal regression to the BOLD signals, QPP1-3 would roughly mirror the patterns 1-3 discovered in (Bolt et al., 2022).

2.1. Software architecture:
Below is an overview of the software architecture:

2.1.1. Prerequisites:
● Software Dependencies: The package requires MATLAB (The MathWorks Inc., Natick, MA, USA, R2018a or a later version) to run. All supporting MATLAB functions needed for the main pipeline are included in the ./QPPv0922/ folder.
● Input Data: The package operates on functional neuroimaging data stored in the ./input/data.mat file. This file needs to include several input variables such as D0, MotionInf, ROI2Net, and NetLB (see Table 1) that are necessary for analysis.

Input variables	Description	Note
D0	a (nsbj X nscn) cell matrix	Each cell has a (nroi X ntimepoints) matrix of EPI timeseries.
MotionInf	a (nsbj X nscn) cell matrix	Each cell includes >=1 segment(s) of timepoints selected for the QPP detection. Timepoints with motion or artifacts can be excluded.
ROI2Net	a (nroi X 1) vector	Each entry is the network index corresponding to each ROI.
NetLB	a (nnet X 1) cell vector	Each cell includes the (shorthand) label of each network.

Table 1: Input variables. nsbj= number of subjects, nscn=number of EPI scans, nroi=number of ROIs, ntimepoints=number of timepoints, nnet= number of networks.

Note that the `ROI2Net` and `NetLB` variables can be generated from your atlas-network file stored in the ./resources/ folder by running 'st0_ROIreOrg.m'. In this case, the EPI data cell matrix should at least be included in your original input file; if you did not prepare the `MotionInf` parameter, the entire timepoints of each scan will be included in `MotionInf` when running 'st0_ROIreOrg.m'.

2.1.2. Main Pipeline:
The main pipeline is divided into three steps:
● Step 1: Setting Parameters (st1_ParamsSet.m): This step involves specifying global parameters for the analysis. Parameters are categorized into various sections, including file paths, QPP global parameters, QPP detection parameters, QPP phase adjustment parameters, and functional connectivity analysis parameters. These parameters determine how the subsequent steps of the pipeline will run. A description of these global parameters, excluding file paths, is provided in Table 2. For an in-depth understanding of each parameter, refer to Table in Section 2.1 of the README manual.

Category	Parameter	Description
QPP global parameters	nP	total number of QPPs to detect
	PL	QPP window length
QPP detection parameters	cth13 & cth45	correlation threshold for different QPPs
QPP phase adjustment parameters	cthph	similarity threshold when phase-adjusting a QPP
	s	control for strict or relaxed phase adjustment
	sdph	reference parcels
Functional connectivity (FC) analysis parameters	fz	control the output FC map to either use Pearson correlation or its Fisher Z-Transformation

Table 2   Global parameters setup in 'st1_ParamsSet.m'

- Step 2: QPP Analysis (st2_QPPanalysis.m): This step is where the actual QPP analysis takes place. It involves detecting and analyzing QPPs based on the specified parameters from Step 1. The script detects QPPs, performs phase adjustment, detects additional QPPs from residuals, and computes functional connectivity after QPP regression. Key output variables such as QPP templates, correlation timecourses, and functional connectivity maps are generated.
- Step 3: Visualization (st3_QPPFCvisual.m): The final step involves visualizing the results of the QPP analysis. This script generates various figures illustrating the detected QPPs, their phase-reversed counterparts, sliding correlation timecourses and their histograms, as well as functional connectivity matrices before and after QPP regression. The script takes parameters for specifying which QPPs and groups to visualize.

2.1.3.   Output Files:

The output files are organized into directories based on the type of analysis performed (GrpQPP, SbjQPP, ScnQPP). Output files include intermediate results as well as key output variables generated during the QPP analysis and visualization steps (described in Section 2.2.2 in the README manual). These variables provide information about detected QPPs, their characteristics, and the results of various analyses. Examples of output files saved by different parameter settings are described in section 3 in the README manual.

Overall, the architecture follows a modular approach, with separate scripts for parameter setting, QPP analysis, and visualization. The input data is read from the specified file, and the analysis results are stored in output files. The package aims to provide a comprehensive tool for researchers to analyze and understand QPPs in functional neuroimaging data.

2.2. Key functions of QPP analysis*:*
The computational framework implemented in the script st2_QPPanalysis.m encompasses a sequence of five analytical procedures designed to extract QPPs and related results present in the data. These five procedures are outlined below.

- *QPP1 Detection:* The initial phase involves the identification of the primary Quasi-Periodic Pattern 1 (QPP1), an intrinsic dynamic phenomenon in the brain. Leveraging

the algorithm developed by (Majeed et al., 2011) and subsequently enhanced by (Yousefi & Keilholz, 2021), this step utilizes a correlation-based approach to detect and separate these phase-locked patterns within a series of chosen timecourses from the brain regions under study. The chosen timecourses are specified in MotionInf as detailed in Table 1.

- *Phase Adjustment*: Based on the findings of (Yousefi & Keilholz, 2021), this stage involves precise phase adjustments to synchronize the phases of QPP1 consistently across all brain regions. During this process, a reference brain region is selected, of which QPP waveform begins from a positive value. This intricate synchronization enhances the comparability of multiple QPPs (e.g., QPP1, QPP2, QPP3, etc.) within a given population.

- *Detection of Additional QPPs (optional):* Extending the analytical framework presented by (Yousefi & Keilholz, 2021), this computation explores residual data following QPP1 regression. The detection of secondary (and potentially tertiary) QPPs from these residuals provides a more comprehensive exploration of this phase-locked intrinsic dynamic process. Parameters for the detection of additional QPPs can be defined within st1_QPPparam.m.

- *Reverse Phase QPP Detection:* Introduced by (Xu, Smith, et al., 2023), this step identifies QPPs in their reverse phase. For each QPP, a counterpart in reverse phase is identified. This reverse phase QPP is derived by averaging segments that initiate from the local minima of the identical correlation timecourse employed to extract the original QPP in either step 1 or 3. This reverse QPP assists in facilitating comparisons due to the half-wave symmetric nature of QPPs as described in (Xu, Smith, et al., 2023).

- *Functional Connectivity Computation after QPP Regression*: Building upon the frameworks of (Abbas, Belloy, et al., 2019b; Xu, Smith, et al., 2023; Yousefi & Keilholz, 2021), this final computation computes the functional connectivity (FC) map from the residue after the QPP regression. By systematically removing QPP-related signals, this analysis unveils refined functional connectivity patterns, implicating the amount of FC contributed by QPPs.

These computations collectively offer a comprehensive toolkit to study QPPs and their contributions in brain functional connectivity. By integrating established methodologies, this analytical framework contributes to advancing our understanding of the intricate spatiotemporal dynamics within the brain data.

3.   Illustrative example
This toolbox has been demonstrated on various datasets with different atlas schemes. Including resting and task human fMRI dataset (Xu, Smith, et al., 2023; Seeburger et al, 2023) as well as multiple rodent fMRI datasets (Xu, Zhang, et al., 2023). One illustrative example of resting fMRI Human Connectome Project (HCP) data extracted from Glasser atlas (Glasser et al., 2016) is provided in this section.

3.1. Prepare the input file
The initial input file should contain a cell matrix of EPI timeseries with dimensions (nsbj X nscn), which can be represented as 'B' in the file './input/B_GSR_HCPR3.mat'. If the remaining variables (MotionInf, ROI2Net, and NetLB) haven not been prepared beforehand, they can be

created using the 'st0_ROIreOrg.m' script. Specifically, the user needs to specify parameters in the script's initial three sections, as illustrated in Figure 1. Note that the atlas spreadsheet (highlighted with blue underscores in Figure 1) must encompass ROI labels and their corresponding functional networks (green circles in Figure 2).

Figure 2   Input variables generation. For demonstration utilizing the Glasser atlas (Glasser et al., 2016), an example screenshot of the variable initialization on MATLAB (left window) and atlas spreadsheet in Excel (right window) is displayed. The initialization variables dataIN, D, D0, and dataOUT need to be properly set. For the specific dataIN file contents, note that the atlas spreadsheet must encompass ROI labels and their corresponding functional networks. The dataIN path and filename are highlighted with blue underscores. The ROI labels and function networks are circled in green. File contents of D where the variable B is located are circled orange. The dataOUT filepath is highlighted with a dark blue underscore.

3.2. Configuring parameters for QPP analysis and visualization

Once the input file is ready, the user will run the script 'st1_ParamSet.m' to set up a range of parameters and thresholds associated with QPP detection, phase adjustment, and network analysis. Each individual parameter is elucidated within the comment lines of the script itself. Additionally, a detailed description of each parameter's role can also be found in the accompanying README manual.

Upon execution of the 'st1_ParamSet.m' script, all of the specified parameters and thresholds are established according to the user's preferences and the specific characteristics of the data. In the context of our example, if the input file is denoted as 'HCPR3gsr' (a file obtained from 'st0_ROIreOrg.m'), the resulting parameters will be saved in a file named 'Param_HCPR3gsr_demo.mat', as indicated in Figure 2A.

Subsequently, the user proceeds to execute the script named 'st2_QPPanalysis.m' to perform the QPP analysis. When running this script, the user's focus is directed solely to the first section, where they can select operational preferences. This is highlighted by a red square in Figure 2B. All resulting output files will be preserved in the designated ./output/ directory.

Finally, the user will execute the script 'st3_QPPvisual.m' to visualize QPP(s) and associated results saved in the ./output/ directory. When running this script, the user still focuses the first section for operational choices (highlighted by a red square in Figure 2C). Note that the operational choices selected in this section and the ones in 'st2_QPPanalysis.m' must be consistent.

A: st1_ParamSet.m   B: st2_QPPanalysis.m

C: st3_QPPvisual.m

Figure 3   Parameter configurations for QPP analysis and visualization. A: Configuration of parameters across all sections of the 'st1_ParamSet.m' script. B: Setup operational choices in the 1st section of 'st2_QPPanalysis.m'. C: Setup operational choices in the 1st section of 'st3_QPPvisual.m'.

3.3. Visualization of final results
The script will automatically produce six distinct figures, each designed for a specific purpose, which includes 1) A visualization depicting the detected Quasi-Periodic Patterns (QPPs); 2) the phase-reversed counterparts of the QPPs that were identified; 3) sliding correlation timecourse depicting the initiation point of the ongoing QPPs.; 4) sliding correlation timecourses between QPP and the whole scan before and after undergoing the QPP regression; 5) histograms portraying the distribution of these sliding correlation timecourses; 6) functional connectivity matrices showcased both before and after the application of QPP regression (see Figure 4).

Figure 4   Six figures generated automatically by the script 'st3_QPPvisual.m'. As an example, these figures show the output from resting fMRI HCP data of two concatenated scans, each encompassing three subjects. Global signal regression was applied to the data in preprocessing. The algorithm utilized a window length of 20s (28 TRs). For each concatenated scan, three QPPs were identified, resulting in three unique patterns: QPP1, QPP2, and QPP3. However, only the results for QPP1 and QPP3 are visualized in each figure. In vertically stacked subfigures, each row represents the results of QPP1 and QPP3 for an concatenated scan. Sequence-wise from the top left to the bottom right, the figure showcases: 1) a depiction of the identified QPPs; 2) the phase-inverted versions of these QPPs; 3) a sliding correlation timeline highlighting the initiation points of the ongoing QPPs; 4) sliding correlation timecourses comparing the QPP to the entire scan pre and post QPP regression; 5) histograms illustrating the distribution of the aforementioned sliding correlation timecourses; 6) a functional connectivity (FC) matrix before QPP regression (upper triangular section) and after QPP regression (lower triangular section) for each detected QPP.

Additionally, users can swiftly visualize the phase-adjusted QPPs or the network-specific QPP waveforms using the command line, as demonstrated in Figure 5, facilitating deeper analysis.

A: QPP template with phase adjustment

B: QPP waveforms averaged across each network

Figure 5   QPPs with adjusted phases. A: the primary and secondary QPP following phase adjustments. In each sub-figure, the QPP of the `ip`-th order, whose phase is aligned based on the `is`-th seed, is displayed using the command: `imagesc(QPPas{ip,1}{is}(iROI2Net,:),[-1 1]);` B: Averaged QPP waveforms across networks for the primary and secondary QPPs with phase adjustments. In every sub-figure, the averaged QPP waveform for the `inet`-th network is illustrated using the command: `plot(mean(QPPas{ip,1}{2}(find(ROI2Net==inet),:)',2));`

4.   Impact

QPPLab is an open-source MATLAB software package, which offers a comprehensive toolset for researchers to study the quasiperiodic spatiotemporal BOLD dynamics for any species. This software introduces several avenues for advancing neuroscience and neuroimaging research and addressing important questions in the field. Firstly, it advances research by providing a user-friendly interface and standardized methodologies for studying QPPs on any fMRI dataset. With QPPs playing a pivotal role in attention (Abbas, Bassil, et al., 2019; Abbas, Belloy, et al., 2019) and arousal fluctuations (Raut et al., 2021), as well as in prevalent brain disorders such as ADHD (Abbas, Bassil, et al., 2019) and Alzheimer's Disease (Belloy, Shah, et al., 2018) across both rodents and humans, this software suite presents a platform to delve into new research inquiries concerning intrinsic spatiotemporal dynamics under novel circumstances. Researchers are empowered to investigate the fundamental mechanisms driving functional connectivity, their contribution in diverse cognitive functions, and brain disorders.

In terms of improving the pursuit of existing research questions, *QPPLab* offers an unprecedented level of comprehensive QPP analysis. By integrating multiple established algorithms and analytical techniques, the software enhances the reproducibility and reliability of QPP detection. This allows researchers to quantitatively assess the extent to which QPPs differ from each other, or contribute to functional connectivity, thus providing insights into the brain's intrinsic dynamic patterns and their functional significance.

The use of *QPPLab* has also changed the common practice of traditional QPP analysis. The software offers an accessible and user-friendly platform for analyzing QPPs, reducing the technical barriers that were introduced by previous study-specific algorithms. By offering a parameter-simplified and user-friendly toolbox, the software streamlines the analysis of QPPs in

diverse datasets. Researchers can now investigate the reproducibility and consistency of QPPs across species and brain regions, shedding light on fundamental principles of brain organization. Published studies utilizing *QPPLab* (Xu, Smith, et al., 2023; Xu, Zhang, et al., 2023) have enhanced the precision and accuracy of QPP detection and analysis, leading to a deeper understanding of brain function.

5. Conclusions

We have presented an open-source and generally applicable MATLAB software package for detecting, analyzing, and visualizing QPPs and other related results from functional neuroimaging timeseries of the brain. *QPPLab* introduced an enhanced algorithm and software, which integrates established methods. The software's interface, designed for accessibility, has expedited analytical processes, thereby fostering rigorous investigations and reproducible outcomes. More importantly, it allows for new investigation into cognitive processes and neurological disorders in humans and other species.

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