Pygoda: A Graphical Interface to Efficiently Visualise and Explore Large Sets of Geolocated Time Series

Abstract

Modern-day data sets in geosciences may comprise hundreds or thousands of geolocated time series. Despite all the automated tools and new algorithms now available to process and prepare those data before using them in research projects, it can be useful or even necessary to visualise and investigate them manually. Whether it be for data quality assessment, for the preparation of a training data set for machine learning, to gain an understanding of the spatio-temporal characteristics of data, or for the inspection of specific observations in a larger data set, there are many cases where an efficient, dedicated tool would be useful for this task. Existing programming languages, libraries and software tend to be either cumbersome to use when aimed at simple visualisation, or lack functionalities when used in more advanced data exploration. Here we present and describe a new software package, Pygoda (doi:10.5281/zenodo.10009814), developed to provide a graphical interface for displaying and interrogating the spatial and temporal components of geolocated time series, offering a comprehensive insight into the data set properties. Time series from hundreds of observation stations can be plotted simultaneously in Pygoda, which comes with a range of functionalities to explore them, both individually or in groups, to extract or compute different parameters from them and use those in sorting and filtering, or to (semi-)manually categorise the records. At the time of writing, Pygoda remains in active development and future user suggestions and contributions are welcome.

Keywords visualisation · time series · geolocated data · data analysis · open source · free software · GUI
1 Introduction

Many research projects in geosciences involve time series acquired at or near the Earth surface. Modern automated tools have enabled us to manage these increasingly large data sets more easily, from their recording to their world-wide sharing. The visualisation of these data and related tasks such as data exploration and quality control is another key issue, which is the main target of the GUI (graphical user interface) software we introduce in this paper. We have named this project Pygoda, a free-form acronym for Python for geoscientific data analysis and visualisation or, alternatively, Python for geolocated time series diagnosis. In order for Pygoda to be both generic and versatile enough, but still appropriate for the task, our focus, for now, is exclusively on geolocated one-dimensional time series; that is discrete observations of a time evolving quantity (the term ‘one-dimensional’ does not preclude the simultaneous observation of several independent components of a vector field).

1.1 Time series and one-dimensional data in geosciences

The sampling of continuous spatio-temporal fields at fixed positions is a routine source of time series in geosciences. These fields are a very common object of study: the Earth’s gravity and magnetic fields, the temperature at Earth’s surface, the crustal velocity field from GNSS, the atmospheric concentration of pollutants, or the geothermal heat flux are only some examples. Time series also result from point observations of processes which are not part of a continuous field, such as river discharges or greenhouse gas emissions. Sources of such data sets are rapidly expanding with the development of the Internet Of Things and citizen science based observations.

Time series come from extremely diverse origins but, in practice, they are first and foremost the same mathematical object, a discrete function of time. Furthermore, from the point of view of geosciences, time series are also similar in terms of processing challenges (including irregular sampling with potential gaps and artefacts such as spikes or steps which have to be corrected, etc.), and in terms of signal content (trend, offsets, noise, tidal and seasonal signal, etc.). Geoscientists are already taking advantage of these similarities by using the same tools across a number of disciplines to process and analyse a wide range of observations. With Pygoda, we aim at going one step further by providing to the scientific community an additional generic and versatile tool to visualise and explore geolocated time series easily, efficiently and flexibly. Admittedly, those terms give latitude for some subjectivity; we will clarify their meaning in the context of this work in the following sections.

Before moving on to a detailed discussion on geolocated time series visualisation, it should be noted that, even if all the examples mentioned in this section come from the geosciences, any observation that is sampled in time and in space at fixed location would fit in the category of data which can be handled by Pygoda. For example, the occurrence of a disease, birth rate or income through time or other socio-demographic properties fall into this class when considered spatially at specific locations. Thus, by providing high-level generic functionalities to visualise georeferenced one-dimensional data, Pygoda could be useful to a wide range of disciplines across the physical, epidemiological and social sciences.

1.2 The challenge and importance of visualisation

The visualisation of georeferenced one-dimensional data is not a new problem. Nevertheless, many data sets have now reached a size where their visualisation has become a challenge in itself, even with the help of digital tools. For example, the Nevada Geodetic Laboratory (NGL) GPS data set contains more than 19 000 unique time series and the European Climate Assessment & Dataset project collects the data from more than 22 000 weather stations in Europe and the Mediterranean regions alone. Even with much smaller data sets, with tens or hundreds of geolocated observations, visualising and exploring them in an efficient way is not a trivial problem.

The main difficulty in the visualisation of geolocated time series is to reconcile geographic plots, which only highlight the spatial variations of the observations, with the conventional plots of one-dimensional data in time domain, which only highlight their time dependency. A few common solutions are used to work around this problem. One of them is to extract a specific feature of each time series in the data set (mean value, trend, maximum value, etc.) and to plot it on a map. The main drawback of this method is a huge loss of information which can hide important and/or valuable spatio-temporal variability or even bias the visualisation if the computed feature is too sensitive to uncorrected artefacts. Another standard approach is to plot successive maps showing the evolution of the observations at all stations. Notwithstanding that this technique enables a simultaneous visualisation of the spatial and temporal dependency of the measured quantity, its main limitation comes from the quantity of information that it may needlessly expose. This approach suffers from the same limitation that it can obscure important and/or useful trends because of

1 http://geodesy.unr.edu/NGLStationPages/GlobalStationList, date consulted: 15/05/2022
2 https://www.ecad.eu/, date consulted: 15/06/2022
the quantity of data displayed and the difficulty in identifying patterns across time-slices. Downsampling is required for long time series unless it is acceptable to use some kind of animation to visualise hundreds of map plots in a short amount of time, which may also suffer from obscuring important underlying behaviours. An additional drawback of this approach is that it is unlikely to reveal interesting spatio-temporal patterns in regions where the data are sparse. In other words, map-based visualisation increases the bias toward densely observed regions to the detriment of poorly observed regions, even when rare but high-quality time series have been recorded in the latter. It is worth noting that both previous visualisation methods are also very sensitive to the data scaling choice and outlier rejection, which is another important reason to be careful when using them.

A last approach is simply to separate the visualisation of the time series themselves and their positions on the map on two different plots. Such an approach has the important advantage of not losing any information, but its use is limited to a small number of simultaneously displayed elements. When thousands of stations are involved in a study, it is already impossible to plot them spatially without cluttering up entire areas and, in any case, only a small number of arbitrarily selected or (hopefully) representative time series can be displayed at the same time.

In such a context, it is tempting to rely on statistics to characterise the content of large data sets – with hundreds or thousands of time series and more – and to come back to in-depth data visualisation only when checking the output of an algorithm against a limited number of selected observations. With the improvement of processing techniques and the emergence of machine learning, it may look like the thorough investigation of larger and larger data set is less of an issue. In terms of data exploration, signal and pattern detection, or data correction, we can now widely rely upon computer capabilities. Data visualisation is still critically needed, however, because many automatic algorithms are not good enough (yet) to be trusted without human input. For example, manual picking of offsets in GPS time series still yields better result than all available automated and semi-automated detection algorithms [Gazeaux et al., 2013, Tehranchi et al., 2020]. Human scrutiny is still needed too where very high accuracy is essential. The last published International Terrestrial Reference Frame (ITRF2014) have involved human intervention to visually inspect the data which went into their realisations [Altamimi et al., 2016]. More generally, quality is better controlled when human operators have a way to efficiently visualise the entire set of observations, especially for comparison purpose and to aid the understanding of common biases, errors or patterns. Last but not least, even when innovative algorithms have the potential to outperform any previous method, visualisation will still be needed at some point. Inverse methods and supervised machine learning are such examples where the quality of an algorithm output depends on human experts who need visualisation tools to prepare the input or training data set. In projects using artificial intelligence techniques, such manual preparation takes up a lot of time [Sun et al., 2022].

1.3 Existing software and a new alternative

The previous discussion has illustrated the importance of data visualisation in general, be it for data exploration, analysis, diagnosis or quality control. Along with the introduction of Pygoda, which was specifically made to tackle those tasks, we also wanted to offer a broad picture of some of the current available tools to visualise geolocated time series and highlight their objective strengths and limitations.

Indeed, numerous high-quality generic tools are available to visualise and analyse one-dimensional data in geosciences but, to the best of our knowledge, none of them is fully dedicated to geolocated time series. When such dedicated tools exist, they are frequently tailored to a specific data set or application and sometimes only provided as an online interface for quick data overview (e.g. the online NGL GPS map³). Our goal here is not to discuss exhaustively the advantages and drawbacks of every available software or programming language in terms of geolocated data visualisation or data analysis. We have only summarized in Tab. 1 the main characteristics of different widespread tools to emphasise the factual limitations of existing solutions and identify possible improvements.

³http://geodesy.unr.edu/NGLStationPages/gpsnetmap/GPSNetMap.html
<table>
<thead>
<tr>
<th>Tools</th>
<th>Capabilities</th>
<th>Main limitation</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>General purpose scientific software and programming language packages</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Matplotlib(^4)/Cartopy(^5) (Python and Julia), ggplot(^6)/tmap(^7) (R), ...</td>
<td>versatile</td>
<td>require coding even for basic visualisation, limited interactivity by default</td>
<td>free, open source; Plotly(^8) is one of the more interactive alternatives</td>
</tr>
<tr>
<td>Matlab(^9), Mathematica(^10), Maple(^11)</td>
<td>versatile</td>
<td>require coding, not available everywhere</td>
<td>proprietary, closed sources</td>
</tr>
<tr>
<td>IDL(^12), GNU Data Language(^13) (GDL)</td>
<td>versatile</td>
<td>require coding</td>
<td>IDL is proprietary, closed source; GDL is a free alternative</td>
</tr>
<tr>
<td>Geographic Information Systems software</td>
<td></td>
<td></td>
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<tr>
<td>QGIS(^14)</td>
<td>geographic data visualisation</td>
<td>geography-oriented, very limited for time series</td>
<td>free, open source</td>
</tr>
<tr>
<td>ArcGIS(^15)</td>
<td></td>
<td></td>
<td>proprietary, closed source</td>
</tr>
<tr>
<td>Miscellaneous tools</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>The Generic Mapping Tools(^16) (GMT)</td>
<td>versatile, scripted data visualisation in geosciences</td>
<td>non-interactive, data analysis is out of scope</td>
<td>free, open source; an API is now available for several languages</td>
</tr>
<tr>
<td>Data science software (Tableau(^17), Plotly Dash(^18))</td>
<td>tailored for complex data visualisation and exploration, ready to use analytics, interactive</td>
<td>unwieldy for simple raw data visualisation and low-level data transformation</td>
<td></td>
</tr>
<tr>
<td>Specialised or semi-specialised tools (see Note for examples)</td>
<td>tailored to a specific community needs</td>
<td>specialisation prevents generic usage</td>
<td>e.g. the Climate Data Store (CDS) toolbox(^19), Tsoft(^20) in gravimetry</td>
</tr>
<tr>
<td>Other online generic tools (Plotly Chart Studio(^21), Tethys Platform(^22))</td>
<td>accessible, interactive, made for sharing results</td>
<td>unusable with large offline data sets</td>
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Table 1: Listing of some well-known tools which are routinely used to visualise and analyse data in geosciences (informally based on the authors’ and authors colleagues’ experience).

Geographic Information Systems (GIS) software are ideal for map creation, sometimes with interactive displays, but they are of limited use for detailed time series analysis and visualisation. Conversely, general purpose scientific software and programming languages with specialised libraries (such as Python, Julia, IDL, Matlab or Mathematica) are by far the most versatile options for time series processing and visualisation but they lag behind GIS software for map display and usually offer non-interactive plots. Such limitations can be overcome thanks to community-developed packages but coding is still needed, which takes time and requires a good knowledge of the packages in use. This is acceptable for dedicated research projects, but not necessarily for quick data visualisation, exploration and quality control. Most other tools are either too specialised or have too broad a scope to replace the previous options. A notable exception might be the Generic Mapping Tools (GMT) which offers both time series and maps visualisation with a high level of control and publication-quality outputs. In addition, GMT can now be interfaced with several

\(^4\)https://matplotlib.org/
\(^5\)https://scitools.org.uk/cartopy
\(^6\)https://ggplot2.tidyverse.org/
\(^7\)https://github.com/mtennekes/tmap
\(^8\)https://plotly.com/graphing-libraries
\(^9\)https://mathworks.com/products/matlab.html
\(^10\)https://www.wolfram.com/mathematica/
\(^11\)https://www.maplesoft.com/products/Maple/
\(^12\)https://www.l3harrisgeospatial.com/Software-Technology/IDL
\(^13\)https://github.com/gnudatalanguage/gdl
\(^14\)https://qgis.org
\(^15\)https://www.arcgis.com
\(^16\)https://www.generic-mapping-tools.org
\(^17\)https://www.tableau.com
\(^18\)https://plotly.com/dash
\(^20\)http://seismologie.oma.be/en/downloads/tsoft
\(^21\)https://chart-studio.plotly.com/create
\(^22\)https://www.tethysplatform.org
of the major scientific programming languages (C/C++, Matlab/Octave, Python, Julia), which means that these tools can complement each other to take advantage of the best of both worlds. The main drawback of GMT remains its non-interactivity which can be a limitation in some use cases, especially when exploring data sets with hundreds of time series and more. Finally and unsurprisingly, a bespoke combination of several of the previous tools typically remains currently the best option to cover most data-related tasks.

Considering those observations and the characteristics listed in Tab. 1, a dedicated piece of software for the visualisation and analysis of geolocated one-dimensional data should:

- be versatile, flexible and cover a wide range of data formats;
- combine time series plotting and map display to properly relate the time and space dimensions;
- provide low-level dedicated functions to extract and visualise a wide range of features from time series (combined analysis and visualisation);
- smoothly handle tens of thousands of recordings stored locally; and
- be interactive, to explore large data sets (thousands of time series) seamlessly.

The previous characteristics are the main guidelines that we have endeavoured to follow during the conception and development of Pygoda. These guidelines have determined most of the general design and key functionalities of Pygoda, and some of our technical choices as well.

2 Pygoda

2.1 General design

Our objective is to make Pygoda evolve and improve with time, taking into account the input of its users. Pygoda is a free open source software distributed under the European Union Public licence (EUPL-v1.2, officially available in 22 languages), which is a European alternative to – and compatible with – the GNU General Public license (GPLv3). In practice, this choice of licence ensures that future improvements of Pygoda will always be shared as free software with the scientific community and beyond.

Its general design should not change dramatically in successive versions, however, because it stems from the essential requirements listed in Sec. 1.3. In the next paragraphs, we will introduce the defining components of Pygoda and their interactions.

2.1.1 Grid of data and maps

The first main component of Pygoda is the grid where synchronised and interactive time series plots are displayed (Fig. 1, G). The main advantage of this grid is that it lets the user visualise many records at the same time without having to explicitly select the data they want to investigate or to manually update a plot repeatedly. On a single standard computer screen, it is possible to show tens of time series simultaneously while keeping a high enough level of detail to identify many features at a glance. By “high enough”, we mean that spikes, offsets, change in trend, etc. might be spotted right from the subplots in the grid, as illustrated by Fig. 1 (G), in which several time series exhibit potentially interesting features which are readily visible at this zoom level. The grid geometry (number of rows and columns) is adjustable: when a more in-depth visualisation is required, only a few time series may be displayed at the same time. If needed, an auxiliary larger plot can also be displayed; it is synchronised with the last hovered or selected time series to provide a plot at higher resolution for further investigation. This zoom plot (Fig. 1, Z) offers a cross-hair for precise value reading and some standard statistics over a user-selected interval. The grid shows successive fixed-size pages which can be quickly skimmed or directly selected through different graphical components (Fig. 1, Gc). With this approach, the user can browse through hundreds to thousands of time series in a few minutes.

The second essential component of Pygoda is its map or, more precisely, its pair of complementary maps, which are synchronised with the grid to display the geolocated stations where the time series have been acquired (Fig. 1, M). Pygoda provides the user with an offline map plotted with the Python Cartopy package for quick and static visualisation

23“free speech”, not “free beer” as the saying goes
25https://www.gnu.org/licenses/gpl-3.0.en.html
Pygoda: a GUI for geolocated time series diagnosis

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Figure 1: Overview of Pygoda main window. G: grid of time series subplots (Gc: essential grid controls, Gf: feature used in display and sorting); M: maps with station locations (Mc: Cartopy-based offline map, Ml: Leaflet-based online map, not displayed here); Z: “zoom plot” of hovered or selected time series; C: category-related controls (Cg: group of categories selection, Ci: interactive category assignment with mouse or keyboard); F: filters for data selection (Fc: category-based filter; Fg: geographic filter); P: auxiliary plots (Pf: features plot). Note that some data, estimated models or categories are random and for demonstration purpose only.

of the entire data set (Fig. 1, Mc), along with an optional online map26, built with the Leaflet library27, for more in-depth and local investigation (Fig. 1, Ml). Synchronisation between the grid and the maps occurs at different level to permanently associate each record with its geographic location without any user intervention. Each time series is linked to a different station with a fixed position. By default, all the stations are plotted on the map but the stations currently displayed in the grid are highlighted for quick identification. When the user browses the grid pages, the map is automatically updated to reflect the current grid state. The grid and the maps are also synchronised: when a station is hovered or selected, either on a map or in the grid, it is instantly highlighted in both figures. It is also possible to switch grid pages simply by clicking on a station on the map. Many other map functionalities are also available, which are detailed in the next paragraphs and sections.

The grid and the maps, and their interactions, constitute the core of Pygoda. On top of them, three essential sets of functions and their associated graphical components improve the visualisation capabilities and provide some useful data selection and analysis tools.

2.1.2 Categories, features, sorting and filtering

The first set of tools provides the concept of category and group of categories for data selection and classification (Fig. 1, C). It lets the user flag a record or assign it to a pre-defined category for further processing or investigation either in Pygoda or with another software. Three categories are available by default: neutral, which is the default category for all stations, good and bad. The user can put a station in the good or bad category in just a key press or mouse click on the grid (Fig. 1, Ci) to keep track of interesting data or exclude bad quality records. It is also possible to select several stations – like a multiple files selection in a GUI file browser – and assign them to a category all at once. The list of stations belonging to each category is automatically saved in text files for easy re-use outside of Pygoda. The user can also create new groups of categories and define additional custom categories for a fine-grained

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26The map itself (the tiles) comes from an online provider such as OpenStreetMap (https://www.openstreetmap.org) and requires a working Internet connection, but data display and user interactions are still handled locally.

27https://leafletjs.com
Pygoda: a GUI for geolocated time series diagnosis

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Figure 2: Pygoda grid and map illustrating category assignment. The subplots and map markers are coloured based on the category of each station in the current group of categories (Behaviour, see top-left combo). The highlighted stations (clear colour) are the ones which are currently selected; they are in the default (neutral) category at the moment. A customisable key press will assign them to a new category and update both the grid and map display using the colour of the chosen category.

classification. These categories are associated with colours which are used both in the grid to quickly identify the time series of a given category and on the maps to colour the stations markers. Having a straightforward way to classify data has many potential applications. As indicated in Sec. 1.2, one of them is the selection of training data for a supervised machine learning algorithm. Another one is the creation of smaller data subsets from a large data set or to identify, for example, “anomalous” or “interesting” stations (as defined by the user) worthy of further investigation.

The second set of tools is built around the concept of data features (Fig. 1, F). A feature is defined as any measure, statistic or characteristic computed for each time series in a data set or extracted from the metadata (station name, station position, etc.). For example, from the time vector of each time series, it is possible to compute the total length of a recording, the number of missing recordings or the longest gap; from the data, the mean value of the observed quantity or the largest offset can be determined; from the station location, a distance to some reference point can be extracted. Arbitrarily more complex computations can also be done. A model can be defined, fitted to each time series and each of the fitted parameters can in turn serve as a new feature. For example, a model with a trend and a seasonal signal can be fitted and the amplitude of the annual oscillation will define a new feature, as illustrated by the red lines in Fig. 3. Many features are already available by default in Pygoda but more will be progressively added. Furthermore, users can define new features as needed: all the data and meta-data can be used in the computation of a feature. In terms of visualisation, computed features are visible both in the grid, as a numerical value displayed on each subplot, and on the map, using a color map to tint the station markers depending on their corresponding feature value. Features are a very powerful tool to quickly identify outliers or to highlight spatial patterns and similarities between stations in a data set. They can also be used as a basis for data classification and category assignment, as described previously. Of course, a feature can also be scientifically interesting in itself, such as the average temperature recorded at a weather station or the trend observed in a gravimetric time series.

The sorting and filtering options are the third set of essential Pygoda tools (Fig. 1, F, Gf and Pf). With them, the user can quickly sort and select stations using arbitrary criteria. Unless stated otherwise, we use the term “filtering” to refer to the selection or exclusion of data based on some criteria, not to the mathematical notion of a filter. Features can be used for sorting (Fig. 3), as mentioned in the previous paragraph, but also for filtering out some time series through a dedicated interface (Fig. 4). Categories is another obvious parameter for filtering (Fig. 1, Fc), but the stations can also be selected based on geographic constraints (Fig. 1, Fg). Stations outside or inside a given geographic area can
Figure 3: Illustration of the computation, sorting and display of time series features in Pygoda. In the grid, a fitted model (linear trend + annual and semi-annual oscillations, red scatter plots) is shown on top of the original time series and, on the map, the markers (stations) are coloured based on the estimated trend. The stations are sorted in reverse order in the grid, showing the stations with the largest trend first. Alternatively, the user could sort by increasing amplitude of annual oscillation, or even sort by time series duration while keeping the same plotted model, in just a few clicks. A zoom of one of the time series is also shown (top-right) after the user has made a quick estimation of its trend over a manually selected period of time.

be easily selected or excluded. The area can be defined by country boundary or custom polygons loaded on the map by the user. The sorting functionality is especially useful when visualising the data in the grid as time series with large similarity (following the sorting criterion) are displayed close to each other. Sorting can also be used to quickly identify a threshold for a feature used in a filter. Overall, sorting and filtering are valuable tools for efficient data visualisation, exploration and selection, which is why they are key functions of Pygoda.

2.2 What Pygoda is not

To avoid any confusion on Pygoda’s goal and anticipate potential users’ expectations, it might be useful to state explicitly what Pygoda is not.

First of all, Pygoda is not and does not provide an API for now. It is a standalone graphical application, not a library of functions which may be called or reused in other projects. This may change in the future, but providing such an API is not currently our main goal or priority.

Secondly, Pygoda is not processing software, and will not let the user modify a data set. Pygoda is meant to be used in a pipeline, with inputs from another software or set of scripts which process the data and possibly convert them into one of the generic file formats readable by Pygoda (if a new file format is required, an extension can be written for it). Pygoda “outputs” can be used as the starting point of further investigations or to prepare a data set for further processing. We write “outputs” in inverted commas because some of Pygoda outputs could be no more than a list of manually selected stations. From this perspective, Pygoda is an efficient, automated way of taking notes when exploring a data set rather than a computing software.

Thirdly, Pygoda is not publication-quality plotting software. Even though it can create a number of valuable plots, including time series, maps and stations distribution based on some selected feature, it is not intended to be used to create high-quality figures. We do not recommend using Pygoda for this purpose as there are a limited number of options to customise the plots and no way to ensure perfect reproducibility of the figures as most of them are automatically updated through user interaction.
Fourthly, Pygoda is probably not the best way to share results with a wide audience. Online tools are likely to be a better option to let anyone quickly visualise a new data set (see Sec. 1.3), unless people interested in the data are willing to install Pygoda on their own computer.

Finally, and on the same topic, currently Pygoda is not able to load data from a remote server unless the data can be made transparently accessible through a locally-mounted virtual drive, an option whose implementation depends on the user operating system. Pygoda can run on a remote computer, however, its graphical interface being forwarded through the network to the user desktop.

2.3 Technical choices and system compatibility

Potential Pygoda contributors may be interested in our technical choices. We refer them to the project repository hosted on GitHub, where a detailed description and justification of such choices are provided, along with more technical information on Pygoda main principles, architecture and overall source code organisation.

Pygoda is mainly written in Python and makes use of a few free software packages and dependencies. One of the advantages of Python is its widespread adoption by the scientific community in recent years, which means that many future users should have the technical knowledge to contribute to Pygoda source code or, at least, read and understand the code, help find bugs and suggest improvements. Specific efforts have been made to provide a self-explanatory and well-documented source code (on which work is still in progress).

Pygoda has been tested on different GNU/Linux distributions, and recent versions of Microsoft Windows. It has also run successfully on a CentOS server with a local display on a Windows desktop PC through X forwarding.

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Figure 4: Illustration of time series filtering based on features in Pygoda. Once a feature has been selected, the user can visualise the time series distribution for this feature and exclude all the stations above/below a selected threshold. This plot is also synchronised with the grid and maps to instantly relates time series, feature value and geolocation.

[Image of a plot showing time series filtering]
3 Illustrative case studies

3.1 GPS time series

3.1.1 Introduction on GPS data

Our first illustrative case study involves a subset of the global NGL GPS data set consisting of about 9,400 daily GPS time series. For the sake of simplicity, we only investigate the vertical component of the displacement here. The input data have been processed to detect and remove offsets with an in-house algorithm. Details about other corrections are not relevant here, but it is worth mentioning that we can toggle these corrections on and off at anytime, which is very useful to visualise their impact on the time series or compare the effect of different corrections.

Our main goal is to clean the data set and check its quality before the next step of our hypothetical study focusing on processes affecting vertical land motion in North America. In the next paragraphs, we describe various common tasks and explain how we accomplish them using Pygoda (we have used Pygoda in similar real world cases in Vishwakarma et al. [2022] and Ziegler et al. [2022]).

The data are stored in a custom HDF5 file whose description is given in the example directory of Pygoda’s GitHub repository. This description is used by Pygoda to load the GPS data set. Fig. 5 depicts the data set loaded in Pygoda. By default, the stations are sorted by name here and the stations whose time series are currently plotted in the grid (first 50 stations here) are displayed with a different marker on the map for quick identification.

3.1.2 Filtering based on station location: North America example

As we are interested in North America, the first step is to exclude all the GPS stations located outside the North American continent (for this demonstration, we include Central America but exclude the Carribean and Hawaii). There are different ways of doing that in Pygoda, the simplest one being to use the default geographic filter to select the stations of interest (Fig. 1, Fg). We open the filter panel and select the regions of interest in the territory hierarchy: we check Canada, the United States (without Hawaii) and the Central America category and apply the selected geographic filter.

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29 https://github.com/yannziegler/Pygoda/tree/master/example
As shown on the updated map, the resulting data set is now limited to 4,300 GPS stations, which are all located in North America (Fig. 6). To avoid doing such a manipulation every time we restart the software, we can export the list of selected stations to a file and use it at startup to only load the stations of interest. In addition, we can now update the map projection in the project configuration file to use a map projection better suited to the North American continent (we use a Lambert Conformal Conic projection on Fig. 7).

3.1.3 Semi-manual time series inspection: offset and trend example

GPS time series can suffer from jumps in measured elevation, known as offsets, due to a variety of causes that may be due to geophysical processes like earthquakes or non-geophysical signals, such as a physical disturbance to the GPS antenna. The NGL data set is provided with a list of potential offset dates, which we have extended with a custom offset-detection algorithm. The result is a list of most, but not necessarily all, offsets for each GPS station, along with a correction, which we have estimated for each GPS time series. Our task now is to assess the quality of the offsets detection and correction algorithms.

We can follow different approaches, including a fully visual and manual checking of the entire data set, which would probably take a few tens of minutes in this case. This is the preferred option if the goal is to prepare a high-quality data set or a data set whose content is very well known. Here, we use a two-step method by first sorting the stations by the size of their largest offset. To do so, we select the “largest offset” feature in the features menu, which will automatically compute the corresponding quantity and sort the entire data set accordingly (see Fig. 1, Gf). We also check the option to sort in decreasing order as we want to see the stations with abnormally large offsets first. The result of this operation is displayed on Fig. 8.

The map has been updated and the stations are now coloured by the value of their largest offset. Now, we can readily identify stations with the largest uncorrected offsets (yellow dots on the map). We then open the Features window to filter out all the stations below that threshold and only keep stations with large offsets (see Fig. 9). The resulting filtered data set comprises a few hundreds stations which we can quickly assign to the custom category “uncorrected offsets” in the dedicated Categories menu. Now, we have a quick way of selecting or excluding all the stations whose time series exhibit one or several undetected or uncorrected offset(s) which we deem too large for our study.

We now need to go a step further by double-checking the time series and adding manually to the “uncorrected offsets” category those stations which went unnoticed in the previous step, while removing from this category the stations which were wrongly included in our selection because of isolated outliers in their time series. To improve our offset
Figure 7: GPS stations in North America after reloading the project with an updated configuration. We now only display North American stations using a Lambert Conformal Conic projection.

Figure 8: GPS time series sorted by largest offset. Note that the largest offset is computed by differentiating the time series, so “offsets” might be due to undetected outliers. For this reason, more work will be required to clean the data set.
detection and correction algorithms, we also need to distinguish stations with detected but poorly corrected offsets from stations with undetected offsets. Once again, we have different ways of accomplishing this task; here we simply go through the data set manually, but we might have fit a model to the time series first (see Sec. 3.1.4) and use the computed (W)RMS (weighted root mean square error) to help in station categorisation. When doing such a manual categorisation, we can either assign the target category to a mouse click (control key + left click on PC) and simply click on the time series in the grid or use the keyboard in interactive mode (by pressing key ‘I’ first or selecting a station with a left click) and assign a category by pressing the number on the keyboard corresponding to the target category (0 is the default/undefined category, 1 is the first category in the list, 2 is the second one, and so on). By default, the next station will be automatically selected once the current station has been assigned to a category. We leave the interactive/selection mode and return to the normal/visualisation mode by pressing the escape key or right clicking on the grid or map.

The previous operations have created text files containing the lists of stations with undetected offsets and uncorrected offsets respectively. These lists can be used outside of Pygoda to improve our algorithms by testing them more specifically against problematic stations. Note that we can compute new offset corrections for the entire GPS data set and simply run Pygoda again afterward without any issue. In this case, there is no need to create a new project and the previously created categories and corresponding lists of stations are preserved. If new corrections are added to the data set instead of replacing old ones, the only requirement is to update the data set description to inform Pygoda that new corrections are available.

3.1.4 Data investigation: hydrology and GIA signals example

Now that we have a cleaner data set, we can investigate the geophysical signals responsible for the observed vertical land motion (VLM). Assume that we are especially interested in VLM due to changes in hydrological loading and/or due to a slow, viscous process called Glacial Isostatic Adjustment (GIA), which is the response of the Earth mantle to past ice loading history. Those processes have been extensively studied both because of their specific interest for geosciences and human societies [Rietbroek et al., 2016, Spada, 2017, Tapley et al., 2019] and because their separation is still an ongoing challenge [Wu et al., 2010, Vishwakarma et al., 2022]. GPS observations are also sensitive to other processes, such as earthquakes and anthropogenic signals, but we will not discuss those in this use case example.

We focus on hydrology first and try, as an example, to qualitatively answer the following question: do we observe a consistent signal across a given region or is there any kind of spatial variation? The region could be defined by
Figure 10: Improving our initial stations categorisation manually. We go through the data set by successively pressing the appropriate number key (1 to put the currently selected station in the “uncorrected offsets” category, 2 for the “over-corrected offsets” category, 3 for “undetected offsets”, and 0 to remove the station from all the categories in the “Offsets” group): the current station is then assigned to the chosen category and the next station is selected. The time series displayed in this example has a large undetected offset (missing vertical blue line on the zoom plot). On this screenshot, we have just moved the station to the corresponding “undetected offsets” category as illustrated by its banana mania colour.

administrative borders, basins, or any other relevant kind of area. Here we look at the Mississippi basin. We start with the clean GPS data set (in which stations from the “undetected offsets” and “uncorrected offsets” categories have been filtered out) and display on the map a new layer containing the main catchments of North America (Fig. 11). Then, we only need to click on the map (middle click on PC) to retain the stations contained inside the selected catchment.

The Mississippi basin contains about 750 GPS stations from our clean data set. We now want to determine how the trend of the time series varies across the basin. To do so, we can fit a predefined model to every time series and sort the stations by their estimated trend. Such an operation is as simple as selecting the trend parameter from the “linear + seasonal” model in the features menu (Fig. 1, Gf) and reverting the sorting order if needed.

The results displayed on the map clearly reveal that the trends are negative in the northern part of the basin whereas they are negligible or slightly positive in the southern part (Fig. 12). The interpretation of this observation is out of scope for this paper, but consistent with what we would expect a-priori, considering the influence of the nearby Great Lakes [Argus et al., 2020]. By default, the estimated model is plotted on top of the time series, qualitatively showing a good fit for most stations here. Of course, we could do a similar investigation using the amplitude of the annual component of the seasonal signal if we are interested in periodic hydrological variations, or we could even use another estimated parameter of another model if the “linear + seasonal” model is too simple for our needs.

Moving to GIA, we can use the same kind of model to estimate the trend for all GPS time series in the rebound region. In North America, the GIA results from the melting of the Laurentide Ice Sheet which covered most of Canada and the northern regions of the United States during the Wisconsin glaciation. Recent GIA models agree that the central part of the bulge with the highest rebound rates is probably located in the Canadian Shield region. Thus, it might be insightful to sort the GPS stations by their distance to some reference point picked in that region, for example in the Hudson Bay area. We do that by pressing control key and middle-clicking on the map (on PC) to define a reference position and selecting the “distance to reference” feature. Then, as we did earlier, we can select the trend parameter from the “linear + seasonal” model in the features menu. Such a visualisation is a neat starting point to investigate the
Figure 11: Pygoda’s map with North America catchments overlay enabled. If a single catchment is selected by clicking on the map, all the stations outside the selected catchment are filtered out and only the stations inside the catchment are displayed (see next figure). Another click reset the filter.

Figure 12: Estimates of the VLM (trends) in the Mississippi catchment. The fitted models (annual and semi-annual oscillations + linear signal) are plotted in red on top of the observed time series; the trend value is displayed under the station names. The negative trends (in blue) are clearly visible in the northern part of the Mississippi basin, whereas stations in the southern part exhibit smaller (in absolute value) or no trends. A few isolated stations have positive trends (in red) and may require further investigation.
Figure 13: VLM due to GIA as seen by GPS. Here we have sorted the stations by distance to a reference point located in the Hudson Bay (which is roughly at the middle of the two GIA main bulges according to GIA models, Peltier et al. [2015], Simon et al. [2017]), while plotting the same fitted models as the one shown Fig. 12.

GIA signal in our GPS data set, identify outliers, assign stations with a GIA-dominant signal to a new “GIA dominant” category or simply and quickly extract a list of stations strongly affected by GIA before further processing.

Much more could be done to explore and investigate this GPS data set in more details using Pygoda’s functionality. In this first use case example, we have offered some insight into Pygoda’s capability and ease of use with realistic tasks that the authors have actually accomplished in their own studies and, which are common in data-based geophysical research.

3.2 River gauge data

3.2.1 Introduction on river gauges data

For our second use case example, we demonstrate the functionality of Pygoda with a slightly different mindset: instead of using the software to achieve a specific aim (quality control, data preparation), here we show how it can be used to investigate the content of a data set with limited preconception. Our goal here is to show Pygoda’s versatility, even though it was initially developed to handle GPS time series.

The second use case involves river gauge data from the RiverLevels.uk website. This website provides data obtained from the UK Environment Agency, which openly shares river levels observations online. River gauges are essential tools to monitor river levels in general and flooding in particular [Hendry et al., 2019, Faulkner et al., 2020]. Almost 3500 river gauges are listed on RiverLevels.uk (mostly in England, Scotland and Wales), but some of them have erroneous metadata or no available data. They are loaded and displayed in Pygoda on Fig. 14.

In the following discussion, we limit the river gauges data set to the English county of Somerset, using the list provided on RiverLevels.uk. This comprises 98 stations, 5 of them with no data (Fig. 15).

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30 https://riverlevels.uk, date consulted: 01/07/2022
31 https://environment.data.gov.uk/hydrology/explore
Figure 14: River gauges time series in the United Kingdom, loaded and plotted in Pygoda. In this section, we use an alternative, light colour theme for Pygoda, whereas all the previous figures with GPS data were using the default dark theme.

Figure 15: Same as Fig. 14, but with the data set restricted to time series from river gauges in Somerset.
3.2.2 Advanced plotting control and subplots synchronisation

As illustrated in Sec. 3.1 figures, GPS time series were similar enough not to require any manual tuning of the plots to visualise them properly. By contrast, the overall shape of raw river gauges time series strongly varies between different stations (Fig. 14), especially because on this occasion we have not undertaken any pre-processing and instead loaded the raw data from their original source. Some time series have large, uncorrected offsets; the amplitude of the variations varies between a few tens of centimeters up to several meters depending on the location; several river gauges have large positive or negative outliers which strongly bias the visualisation and even the shape of the variations (seasonal variation, flooding or other events) widely varies. As a result, it is hard to visually inspect or compare the river gauges time series when plotted all together in the grid.

Pygoda provides a set of controls to specifically tackle this kind of grouped visualisation problem. Both the x-axis (time range or t-range) and y-axis (y-range) can be synchronised between all the subplots. By default, each time series is plotted from its first to its last data point. When the t-range synchronisation is enabled, the start and end dates are the same for all the subplots (this option is already enabled on Fig. 15). The y-range can be synchronised similarly, but many more options are provided to adapt the synchronisation to the specificity of each data set. The base or reference level of all the time series can be set – zero (by default), the first value of the time series, its median, its mean, etc. – as well as the lower and upper bounds. Different types of bound are provided to accommodate a wide range of time series: ‘absolute’ (by default, to refer to the data value below/above the reference), ‘percentile’ (to plot a percentile of the data below/above the reference level), ‘sigma’ (bounds are multiples of $\sigma$, the standard deviation) and a few others.

Here we would like to ignore outliers when visualising the time series and make the variations as visible as possible because, for now, we are more interested in the shapes of those variations than in their amplitudes. To do so, we set the reference level to ‘median’ to roughly center the time series vertically in each subplots and set the type of bounds to ‘percentile’. After some trial and error, setting the y-range lower bound to $-97\%$ and the upper bound to $98\%$, give us the plots shown on Fig. 16, which should be compared with the original, default set of plots on Fig. 15.

The variations for most if not all of the time series are now clearly visible and we can readily identify stations with unusual variations. In particular, it now becomes obvious that some river gauges are actually used as tide gauges, recording the tidal cycle in the Severn Estuary and Bristol Channel, as confirmed by the station name (for some of them) and their location on the coast.

Figure 16: Same as Fig. 15, but with a custom, synchronised y-range which improves the visualisation and comparison of time series variations.
3.2.3 Leaflet map specific features

The default, Cartopy-based map of Pygoda we used in Sec. 3.1 is adapted to the visualisation of geolocated time series over a large area (e.g. at continental scale). Here, we are visualising measurements made over an area of about 4,000 km$^2$, which makes the use of a large scale map less practical. This is a situation where the alternative, online, Leaflet-based map of Pygoda might be better-suited.

With river gauges in particular, it makes sense to visualise the river path and local environment along with the recorded water level. Such functionality is offered by the interactive online map of Pygoda, which can display detailed geographic information at local scale as illustrated on Fig. 18, or even online satellite imagery.

It is also possible to use the online map exclusively for users who would like an interface similar to the online visualisation tool of the NGL (for GPS time series, see Sec. 1.3), where a single click on a station opens a popup with the corresponding time series (see Fig. 19).

3.2.4 Zoom plot functionality

The last set of functionality to demonstrate is related to the zoom plot (Fig. 1, Z). This plot provides a crosshair for quantitative data investigation through simple measurements. By default, the crosshair is snapped to the closest data point when hovering the zoom plot, but keeping a key pressed can snap it either to the closest date (ctrl + hover on Windows) or closest data point in amplitude (shift + hover on Windows).

Simple statistics on the time series are automatically computed when the user defines an interval by selecting two data points (start date and end date) successively. Here for example, we can select the starting date of a rise in a river level to define the beginning of an interval, then select the end date of the event to finish the interval selection. As a result, information is displayed on the zoom plot about the duration of the selected event, its amplitude, an estimate of the trend and a few other parameters (see Fig. 20).

The selected interval is set globally, which means that when other stations are hovered or selected, the same information are provided on the same interval. This lets the user readily compare the signal on the same time period across different stations. Thus, with river gauges, we can compare the amplitude of an event at successive gauges along...
Figure 18: Same as Fig. 16, but we now use the online Leaflet map to visualise the river gauges position. Now rivers are visible and stations location can be checked with high accuracy.

Figure 19: “Fullscreen” visualisation (the Leaflet panel has been resized to occupy most of the screen space) of river gauges time series directly on the Leaflet map. This way of using Pygoda might appeal to users who are familiar with map-based online visualisation tools.
the same river, or investigate the time delay between the appearance of a given event in observations made at nearby stations.

4 Conclusion

Pygoda is a new free, open source software tool that has been developed to visualise and explore geolocated time series. It was specifically designed to make common and/or repetitive tasks less time-consuming, and requiring less specific, technical skills to let the user focus on data analysis. Minimal effort is required to import and work on data sets in Pygoda, and this should be improved as Pygoda is further developed. Its long-term goal is not to fully replace other scientific software, but to usefully complement them in traditional workflows. As such, and even though it was initially aimed at geoscientists, Pygoda could be of interest to a large community of users.

Pygoda remains in active development and many improvements are already planned. A roadmap is provided in the project repository but user suggestions and contributions are welcome. We have provided an overview of Pygoda’s main functionalities in this document; more technical information, further explanations and the documentation (in progress) are available on the software repository.

Computer Code Availability

Pygoda is published under the European Union Public licence version 1.2 (EUPL-v1.2)32. The software, source code and basic instructions are all available on Pygoda’s GitHub repository: https://github.com/yannziegler/Pygoda. Issues encountered while using the software should be submitted here as well. Detailed documentation for both users and contributors is available at https://pygoda.readthedocs.io/. If you use Pygoda, please cite it using DOI:10.5281/zenodo.10009814.

Authorship statement

YZ designed and developed the software, and wrote the original version of the manuscript. JB provided the funding within the GlobalMass project, tested the software before its public release and contributed to the manuscript.

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