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ErrUncSeriesAnalyzer: ERROR AND UNCERTAINTY SERIES ANALYZER

1. Introduction

Mathematical models are simplified representations of real-world systems, structured to extract information, characteristics, and behavioral patterns from complex systems (Wess et al., 2021). These models rely on mathematical equations to describe phenomena of interest (Souza et al., 2011), which are solved based on predefined coefficients and observed data.

In environmental studies, mathematical modeling plays a pivotal role in understanding and predicting changes in ecological, climatic, and hydrological systems. Among these applications, hydrological models stand out as mathematical representations of water flow within the hydrological cycle, encompassing interactions between the atmosphere, surface, and subsurface at the watershed scale. These models are widely used to address practical challenges such as water balance analysis, pollutant transport, erosion processes, sediment discharge and deposition, and rainfall-runoff relationships (Ferreira et al., 2021).

The selection of an appropriate hydrological model depends on the specific purpose of the analysis. These models are applied in diverse areas, including water resource management, flood forecasting, agricultural planning, and climate change impact assessment. Their value lies in their ability to simplify complex processes into actionable insights, thereby supporting informed decision-making.

Evaluating the performance of hydrological models requires robust error metrics to quantify the accuracy of simulations against observed data. Commonly employed metrics, such as BIAS, Percent BIAS (PBIAS), Root Mean Square Error (RMSE), Mean Absolute Error (MAE), correlation coefficient (R), coefficient of determination (R^2), and Nash-Sutcliffe Efficiency (NSE), are crucial for identifying overestimation or underestimation trends (BIAS and PBIAS), measuring error magnitudes (RMSE and MAE), and assessing model correlation and overall efficiency (R, R^2, and NSE).

The choice of efficiency criteria significantly influences the evaluation of hydrological model performance, as it affects the model results due to variability, outliers, and bias. Understanding these metrics is crucial for addressing uncertainties related to calibration in hydrological predictions (McInerney et al., 2024). Similarly, selecting appropriate evaluation metrics is critical because they significantly impact both model calibration and performance assessment (Zhao et al., 2024).

However, accuracy alone is insufficient to ensure the reliability of hydrological models. It is imperative to address the challenges posed by uncertainties, which arise from various sources, including errors in input data, limitations in parameter calibration, and simplifications of physical processes. These uncertainties directly impact the credibility of model predictions, underscoring the need for robust methods to quantify and communicate the variability associated with model outputs.

Approaches such as the 95% Prediction Uncertainty (95PPU) band analysis offer an effective solution by quantifying the variability in model predictions. Tools like SWAT-CUP, specifically developed for the SWAT model, integrate error metrics with 95PPU analysis, providing a more comprehensive evaluation of model performance and uncertainties (Abbaspour, 2015). However, this methodology remains confined to SWAT, limiting its applicability to other hydrological models that could equally benefit from such an approach. Additionally, conducting these analyses often requires advanced programming expertise in languages such as Python or R, which may pose a barrier for non-specialist practitioners.

The lack of flexible and accessible tools for performing 95PPU uncertainty analysis across different hydrological models further restricts comparability between modeling approaches. This highlights the need for solutions that expand the scope of performance and uncertainty analysis while lowering technical barriers to their adoption.

To address these gaps, this study introduces the ErrUncSeriesAnalyzer, a software tool designed to extend performance and uncertainty analysis to various hydrological models. The choice of Python as the development language was driven by its widespread adoption within the scientific and technological communities, its versatility, and its extensive library ecosystem for data analysis, mathematical modeling, and graphical user interface development. Moreover, Python facilitates a collaborative environment with a large global network of users, enhancing the tool's support and scalability.

The ErrUncSeriesAnalyzer was developed to be accessible and flexible. Built on Python 3 and compatible with 64-bit Windows 10/11 systems, the tool eliminates the need for advanced programming knowledge through its user-friendly graphical interface. It calculates error metrics (BIAS, PBIAS, RMSE, MAE, R, R^2, and NSE) and performs 95PPU uncertainty analysis using CSV files containing simulation results.

A distinguishing feature of the ErrUncSeriesAnalyzer is its availability as a free-access tool. The executable is hosted on GitHub, making it freely accessible to researchers and practitioners. This approach provides a practical and accessible solution for users.

By enhancing accessibility and enabling comparative analyses, the ErrUncSeriesAnalyzer represents a significant advancement in the evaluation of hydrological model performance and uncertainties. Its application can support critical areas such as assessing climate change impacts on watersheds, planning water supply systems, and mitigating floods, thereby strengthening the scientific basis for environmental decision-making and benefiting both the academic community and professional practitioners.

2. Error metrics

After the preparation of input data, the definition of scenarios, and the execution of simulations, it is essential to assess the quality of the results – essentially, verifying how well the model has been able to represent the phenomenon under study. There are several performance metrics available in the literature for comparing predicted and observed time series. Generally, these metrics are calculated based on the residuals generated by the differences between these series. This section discusses the commonly used metrics in hydrological studies.

The NSE coefficient is the most used performance indicator to assess predictive capability in hydrological models (Ferreira et al., 2020). This index is calculated as the ratio between the variance of the error in the modeled time series and the variance of the observed time series. It can be applied in various contexts, including as an objective function in calibration models (e.g., in the SWAT-CUP calibration software) or for comparing time series to obtain a goodness-of-fit score (Abbaspour, 2015). The value ranges from 0 to 1, where 1 indicates the best fit. However, the interpretation of the index varies according to different authors. For Almeida et al. (2018), values below 0 are considered inappropriate; between 0 and 0.36, the fit is poor; between 0.36 and 0.60, the fit is satisfactory; between 0.60 and 0.75, the fit is good; between 0.75 and 1, the fit is very good. Ahmad et al. (2019) interpret values below 0.3 as inappropriate; between 0.3 and 0.5 as satisfactory; between 0.5 and 0.7 as good; and between 0.7 and 1 as very good. According to Moriasi et al. (2015), NSE values greater than 0.80 are considered very good, between 0.70 and 0.80 are good, between 0.50 and 0.70 are satisfactory, and values below 0.50 are unsatisfactory. This classification by Moriasi et al. (2015) provides a widely accepted framework for evaluating model performance in hydrological simulations, further highlighting the importance of the NSE coefficient in assessing predictive accuracy. The equation for NSE is given by

$$NSE = 1 - \frac{\sum_{i=1}^{n}\left(Q_{sim(i)} - Q_{obs(i)}\right)^2}{\sum_{i=1}^{n}\left(Q_{obs(i)} - \bar{Q}_{obs}\right)^2} \tag{1}$$

where, n is the analysis period (interval); $Q_{sim(i)}$ is the simulated parameter at step i; $Q_{obs(i)}$ is the observed parameter at time step i; and $\bar{Q}_{obs}$ is the mean of the observed series.

The PBIAS measures the average tendency of the modeled values to be either higher or lower than the observed values, expressed as a percentage. It is widely used in hydrological models (Dhami et al., 2018). Like the NSE, this metric is also used as an objective function in SWAT-CUP for model calibration, as well as comparing modeled and observed time series based on a percentage score (Abbaspour, 2015). The ideal value for PBIAS is 0, which indicates no bias. The interpretation of PBIAS is as follows: values greater than |50%| are considered inappropriate; between |25%| and |50%|, the fit is poor; between |15%| and |25%|, the fit is satisfactory; between |10%| and |15%|, the fit is good; and between 0 and |10%|, the fit is very good. According to Moriasi et al. (2015), a PBIAS value of less than 5% is considered very good, between 5% and 10% is good, between 10% and 15% is satisfactory, and values greater than 15% are considered unsatisfactory. This classification allows for an effective assessment of model bias in hydrological simulations, reinforcing the significance of PBIAS in ensuring model accuracy. The equation for PBIAS is given by

$$PBIAS = 100 * \frac{\sum_{i=1}^{n}\left(Q_{sim(i)} - Q_{obs(i)}\right)}{\sum_{i=1}^{n} Q_{obs(i)}} \tag{2}$$

The RMSE is a positive indicator, expressed in the unit of the analyzed parameter, that represents the magnitude of the error between the series. A value of 0 indicates a perfect fit between the series. The squared component of the formulation penalizes peaks by squaring the outliers, thus reflecting the magnitude of the error. While the RMSE is presented in the unit of the parameter, it does not follow any specific scale and depends on the phenomenon under study as well as the modeler's interpretation. It is often used as a component of other indicators, such as the RSR (Ferreira et al., 2020). The equation for RMSE is given by:

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(Q_{sim(i)} - Q_{obs(i)}\right)^2} \tag{3}$$

The R^2 is a measure of the goodness of fit of the regression model, ranging from 0 to 1, and quantifies the percentage of the variation in the simulated data explained by the observed data. According to Almeida et al. (2018), R^2 is interpreted as inappropriate for values below 0.25; poor between 0.25 and 0.5; satisfactory between 0.5 and 0.6; good between 0.6 and 0.75; and very good between 0.75 and 1. R^2 is also used as an objective function in SWAT-CUP calibration models (Abbaspour, 2015). Moreover, Moriasi et al. (2015) proposed a classification system for R^2 values, where values greater than 0.85 are considered excellent (very good), values between 0.75 and 0.85 are considered good, values between 0.60 and 0.75 are satisfactory, and values below 0.60 are deemed unsatisfactory. This dual interpretation from Almeida et al. (2018) and Moriasi et al. (2015) allows for a more nuanced assessment of model performance, helping to define how well the model represents the observed data variability.

$$R^2 = \left(\frac{\sum_{i=1}^{n}\left(Q_{obs(i)}-\underline{Q}_{obs}\right)\left(Q_{sim(i)}-\underline{Q}_{sim}\right)}{\sqrt{\sum_{i=1}^{n}\left(Q_{obs(i)}-\bar{Q}_{obs}\right)^2 * \sum_{i=1}^{n}\left(Q_{sim(i)}-\bar{Q}_{sim}\right)^2}}\right)^2 \tag{4}$$

where, $\bar{Q}_{sim}$ is the mean of the simulated series.

The R measures the degree of linear correlation between two series, assessing the behavior of the curves. The index ranges from -1 to 1, with 0 indicating no linear correlation, 1 indicating a perfect positive linear correlation, and -1 indicating a perfect negative linear correlation. According to Sales et al. (2021), the interpretation is as follows: insignificant correlation between 0 and |0.1|; low between |0.1| and |0.39|; moderate between |0.4| and |0.69|; high between |0.7| and |0.89|; and very high between |0.9| and |1|. The equation for the correlation coefficient is given by:

$$R = \frac{\sum_{i=1}^{n}\left(Q_{obs(i)}-\underline{Q}_{obs}\right)\left(Q_{sim(i)}-\underline{Q}_{sim}\right)}{\sqrt{\sum_{i=1}^{n}\left(Q_{obs(i)}-\bar{Q}_{obs}\right)^2 * \sum_{i=1}^{n}\left(Q_{sim(i)}-\bar{Q}_{sim}\right)^2}} \tag{5}$$

The BIAS or MBE, also known as the average systematic error, is obtained by calculating the difference between the simulated and observed series, expressed in the unit of the phenomenon. This characteristic allows for negative values, indicating whether, on average, the model tends to underestimate or overestimate the parameter being analyzed. A value of 0 indicates a perfect fit with no bias toward overestimation or underestimation. The equation for BIAS is given by:

$$BIAS = \frac{1}{n}\sum_{i=1}^{n}\left(Q_{sim(i)} - Q_{obs(i)}\right) \quad (6)$$

The MAE measures the absolute distance between each pair of observed and predicted values, providing an average score over the entire time series. This metric dilutes the impact of outliers, offering a better fit compared to RMSE. Like RMSE, MAE is presented as a positive value, with 0 indicating the best fit. The closer the RMSE is to the MAE, the less significant the deviations in peaks and valleys. The equation for MAE is given by:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|Q_{sim(i)} - Q_{obs(i)}\right| \quad (7)$$

These metrics are essential tools for evaluating and comparing the performance of hydrological models, providing insight into how accurately the model represents the studied phenomena.

3. Uncertainty: 95PPU calculation

This methodology, inspired by Abbaspour (2015), determines the uncertainty bands based on the 2.5th and 97.5th percentiles of behavioral simulations, capturing the range of potential streamflow outcomes influenced by parameter variation.

The uncertainty analysis for the simulation-based time series begins with sorting the data in ascending order for each time series. Let X_i represent the raw time series data for the $i-th$ simulation, where the data points are denoted as $x_{i1}, x_{i2}, \dots, x_{in_i}$, and n_i represents the total number of data points in the series. After sorting, we obtain X_i^{sorted}, which is the time series data sorted in ascending order such that $x_{i1} \leq x_{i2} \leq \cdots \leq x_{in_i}$. This sorting is essential for determining the intervals and subsequently calculating the distribution.

Next, we define the interval size Δ_i for each time series. The interval size is calculated by dividing the range of the sorted data by the number of bins, which is set to 10. Mathematically, this is expressed as:

$$\Delta_i = \frac{max\left(X_i^{sorted}\right) - \min\left(X_i^{sorted}\right)}{10} \tag{8}$$

where: $max\left(X_i^{sorted}\right)$ and $\min\left(X_i^{sorted}\right)$ represent the maximum and minimum values of the sorted data, respectively. The denominator, 10, refers to the number of bins used for dividing the data into intervals.

In addition to the interval size, we calculate half of the interval size, denoted as $\Delta_{i,half}$. This value is used to define the first value of the intervals. It is computed as:

$$\Delta_{i,half} = \frac{\Delta_i}{2} \tag{9}$$

To construct the intervals, we define P_i as the sequence of interval boundaries for the $i-th$. The first interval begins at the minimum value of the sorted data, and subsequent intervals are generated by adding Δ_i iteratively. Mathematically, this is formulated as:

$$P_i = \{\, p_{i,k} | p_{i,k} = \min\left(X_i^{sorted}\right) + k.\Delta_i,\ \mathrm{k} = 0, 1, \dots, 10\} \tag{10}$$

Where, $p_{i,k}$represents the $k-th$ boundary of the intervals, with k indexing the boundaries from 0 to 10. The intervals are inclusive on the lower bound and exclusive on the upper bound.

Following the interval definition, we calculate the frequency distribution for each time series, represented by F_i. This distribution is determined by applying a histogram function to the sorted data X_i^{sorted} using the intervals P_i. The frequency distribution is computed as:

$$F_i = histogram(X_i^{sorted}, P_i) \tag{11}$$

After calculating the frequency distribution, we compute the total number of observations T_i for the $i-th$. This is simply the sum of all the frequencies in F_i, expressed as:

$$T_i = \sum_{j=1}^{10} F_{ij} \tag{12}$$

Where, F_{ij} is the frequency of data points in the $j-th$ interval for the $i-th$ simulation.

Subsequently, we compute the percentage distribution, denoted as $P_{d,i,j}$, which represents the proportion of data points in each interval as a percentage of the total observations. This is given by:

$$P_{d,i,j} = \frac{F_{ij}}{T_i} x100 \tag{13}$$

where, $P_{d,i,j}$ is the percentage of data points in the $j-th$ interval for the $i-th$ simulation.

To calculate the cumulative percentage distribution, we define $P_{cd,i,j}$ as the cumulative sum of percentages up to the $j-th$ interval:

$$P_{cd,i,j} = \sum_{k=1}^{j} P_{d,i,k} \tag{14}$$

Finally, the ratio r_i for each interval is calculated, representing the change in cumulative percentage distribution between successive intervals, normalized by the size of the interval. The formula for the ratio is:

$$r_{i,j} = \frac{P_{cd,i,j+1} - P_{cd,i,j}}{P_{i,j+1} - P_{i,j}} \tag{15}$$

where, $P_{i,j}$ represents the lower boundary of the interval $j-th$ within the set P_i.

After these calculations, the uncertainty bounds, $L95PPU$ and $U95PPU$, are computed. These bounds represent the 95% prediction interval for the simulation data. The lower bound $L95PPU$ is calculated using the following equation:

$$L95PPU = P_{i,0} + \frac{2.5 - P_{cd,i,0}}{r_{i,0}} \tag{16}$$

$$U95PPU = P_{i,10} + \frac{97.5 - P_{cd,i,10}}{r_{i,10}} \tag{17}$$

The mean of bandwidth, denoted as $\mu_{Bandwidth}$, is a measure of the width of the uncertainty distribution. It is calculated by the difference between the upper and lower limits of the 95% prediction interval of the uncertainty, normalized by the variation in the cumulative distribution. This mean is given by:

$$\mu_{Bandwidth} = \frac{1}{n} \sum_{i=1}^{n} (U95PPU_i - L95PPU_i) \tag{18}$$

Subsequently, the r-factor can be normalized by the standard deviation of the observed data, adjusting the magnitude of the uncertainty in relation to the variability of the real data. This normalization is given by dividing the mean bandwidth by the standard deviation (σ_{obs}) of the observed data:

$$rfactor = \frac{\mu_{Bandwidth}}{\sigma_{obs}} \tag{19}$$

On the other hand, the p-factor measures the proportion of observed errors that fall within the 95% prediction interval of the uncertainty. For each time step i, the p-factor is defined by the following indicator function, which assumes the value 1 if the observed error is within the 95% uncertainty interval, and 0 otherwise:

$$p_i = \begin{cases} 1\ if\ LERROR_i \leq U95PPU_i\ and\ UERROR_i \geq L95PPU_i \\ 0 \end{cases} \tag{20}$$

where, $LERROR_i$ and $UERROR_i$, represent the lower and upper bounds of the observed error for time step i.

The observed error bounds for each time step i are given by:

$$LERROR_i = OBS_i - OBS_i * uncertatinty_{obs} \tag{21}$$

$$UERROR_i = OBS_i + OBS_i * uncertatinty_{obs} \tag{22}$$

where, OBS_i is the observed value for time step i, and $uncertatinty_{obs}$ is the error rate associated with the observed data. This $uncertatinty_{obs}$ value is defined by the user and denotes the uncertainty measurement.

Finally, the p-factor is given by:

$$pfactor = \frac{\sum_{i=1}^{n} p_i}{n} \tag{23}$$

4. Installation

- Downloading the Executable:
  1. Access the download link (item 7.2.9).
  2. Extract the executable files to a folder of your choice.

- Initial Setup:
  3. No software installation is required. Simply run the downloaded file.

5. System Requirements
   - Operating System: Windows 10/11 64-bit

6. Main Features and Workflow
   - Performance Calculation: Supports RMSE, MAE, BIAS, PBIAS, R, R^2, and NSE as objective functions.
   - Uncertainty Calculation: Uses 95PPU, R-Factor, and P-Factor theory.
   - Data Import: Imports simulation data from a CSV file.
   - Data Export: Exports results to an Excel report (.xlsx).
   - Plotting: Generates and exports plots of the results.

The operational algorithm (Fig. 1) ensures precise processing from data importation to final export, supporting robust scientific analysis and streamlining workflows for water resource studies.

7. User Interface Overview

The main window (Fig. 2) consists of several sections:

- Import Section
  - File Name Input: Input field for the CSV file name.
  - Browse Button: Opens a file browser to select the CSV file.
  - Import Button: Imports the selected CSV file.
  - Read Button: Reads and displays the data from the CSV file.
- Error Calculation Section
  - Objective Function Selection: Radio buttons to select the desired objective function (BIAS, PBIAS, RMSE, MAE, r, r^2, NSE).
  - Calc Error Button: Calculates errors based on the selected objective function.
  - Error Table Button: Displays a table of calculated errors.
  - Best Simulation Button: Displays the best simulation based on the selected objective function.

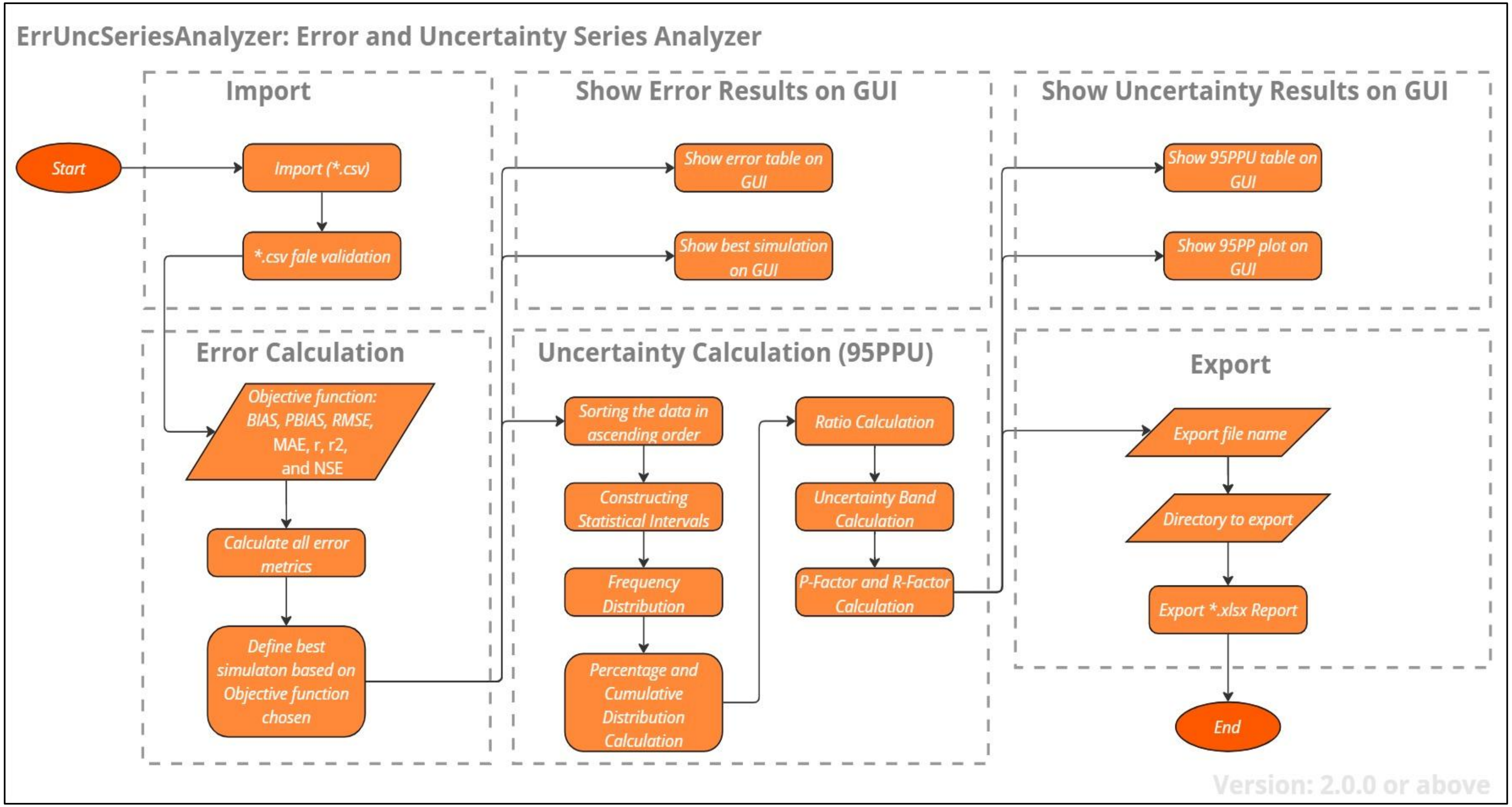

Fig. 1. ErrUncSeriesAnalyzer operational algorithm.

- Uncertainty Calculation Section
  - Error in Observed Input: Input field for the error in observed values.
  - Uncertainty Calc Button: Calculates uncertainties.
  - Read Uncertainty Button: Displays a table of calculated uncertainties.
  - View Plot Button: Displays a plot of uncertainties.
- Export Section
  - Export File Name Input: Input field for the export file name.
  - Export Directory Input: Input field for the export directory.
  - Folder Browse Button: Opens a folder browser to select the export directory.
  - .xls Report Button: Exports results to an Excel file.

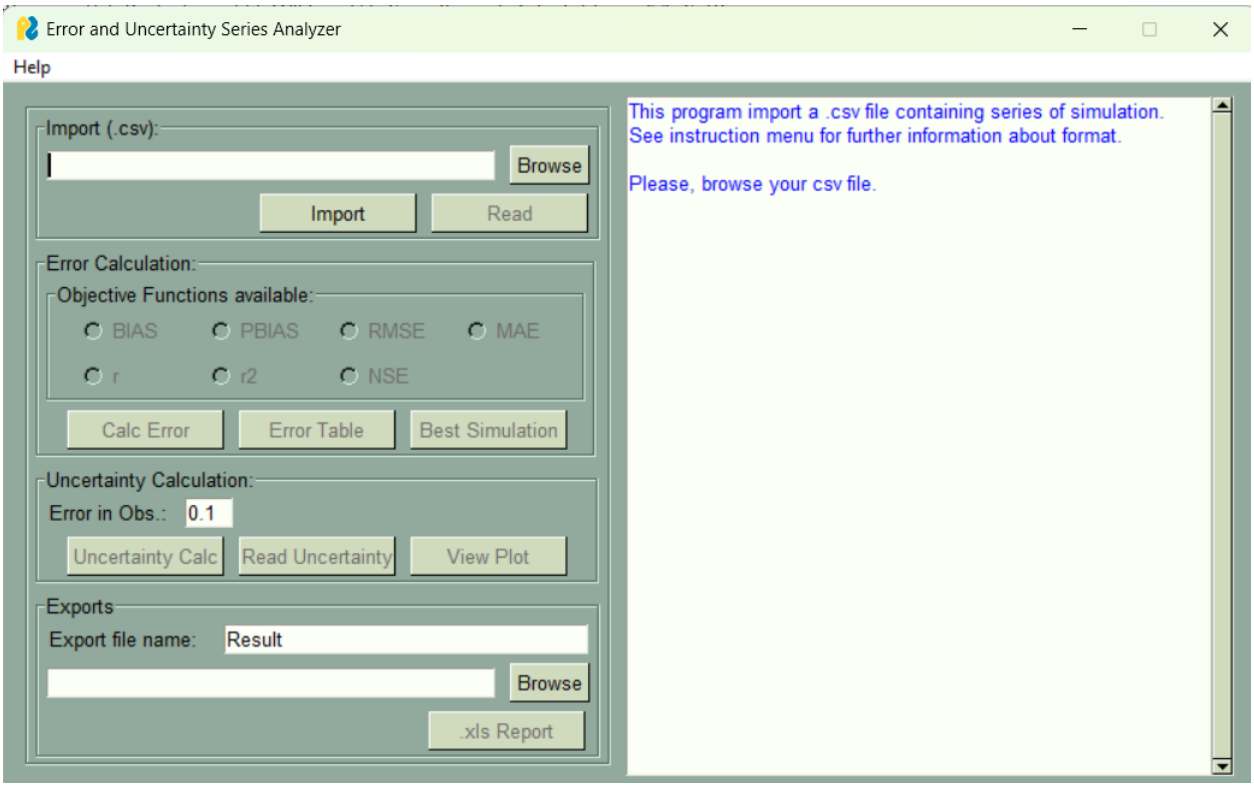

Fig. 2. ErrUncSeriesAnalyzer user interface.

8. Input Table Requirements

- CSV file with data from simulations.

Date	Observed	SIM1	SIM2	SIM3	SIM4	SIM5	…
01/01/2008	6.5699	9.14	11.18	11.5187	12.3320	13.32	…
02/01/2008	6.5699	8.85	10.72	10.9041	11.6228	12.58	…
03/01/2008	6.098	8.06	9.9	10.0471	10.7403	11.71	…
…	…	…	…	…	…	…	…

Notes

- Ensure the CSV file follows the correct format: The first column must be the date, the second column must be the observed data, and subsequent columns are the simulation data.
- The CSV file should not contain NaN values, and all series must have the same dimensions.
- The separator used should be ';'.
- An example.csv (example_csv_file.csv) file is provided with program exe.

Note: It is not allowed NaN values in the series and all series (columns) must have the same dimensions.

9. Links

Repository:

https://github.com/dhiegosales/ErrUncSeriesAnalyzer

User manual:

https://github.com/dhiegosales/ErrUncSeriesAnalyzer/blob/main/README.md

Releases:

https://github.com/dhiegosales/ErrUncSeriesAnalyzer/releases

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