Getting Started with GPCurvist 1.0

📄 Data

GPCurvist 1.0 uses a **built-in data entry table**

Use the **"Data Entry"** panel on the right side of the main window.
• Manually type or **paste** your data into the table.
• Each row represents one observation (replicate)

You can manage the table by right-clicking to paste data, add or remove rows, or use **Ctrl+V** to paste directly.

💡 Tips:

For the analysis to run correctly, **every cell must have a valid entry**:
• No empty cells
• No missing or invalid numbers
• No text in numeric columns (X and Y)
• The first column (Sample_name) must contain at least one character, such as A1, A2, Sample1, or Sample2

If cells are empty or invalid, the app will either:
▪ Show an error message, or
▪ Return inaccurate or failed calculations.

✅ Best Practices

• Use **at least 5 levels of time and 4 replicates per group** for better modeling accuracy
• Use the **"Clear Data"** button to reset the table
• Always check your table for complete, valid entries before clicking **"Run Analysis"**

User guide for GPCurvist

When starting **GPCurvist.exe**, a window (Figure 1) will appear where the user is required to enter several values before running the model. These values are necessary for customizing the neural network and data processing pipeline for your specific dataset.

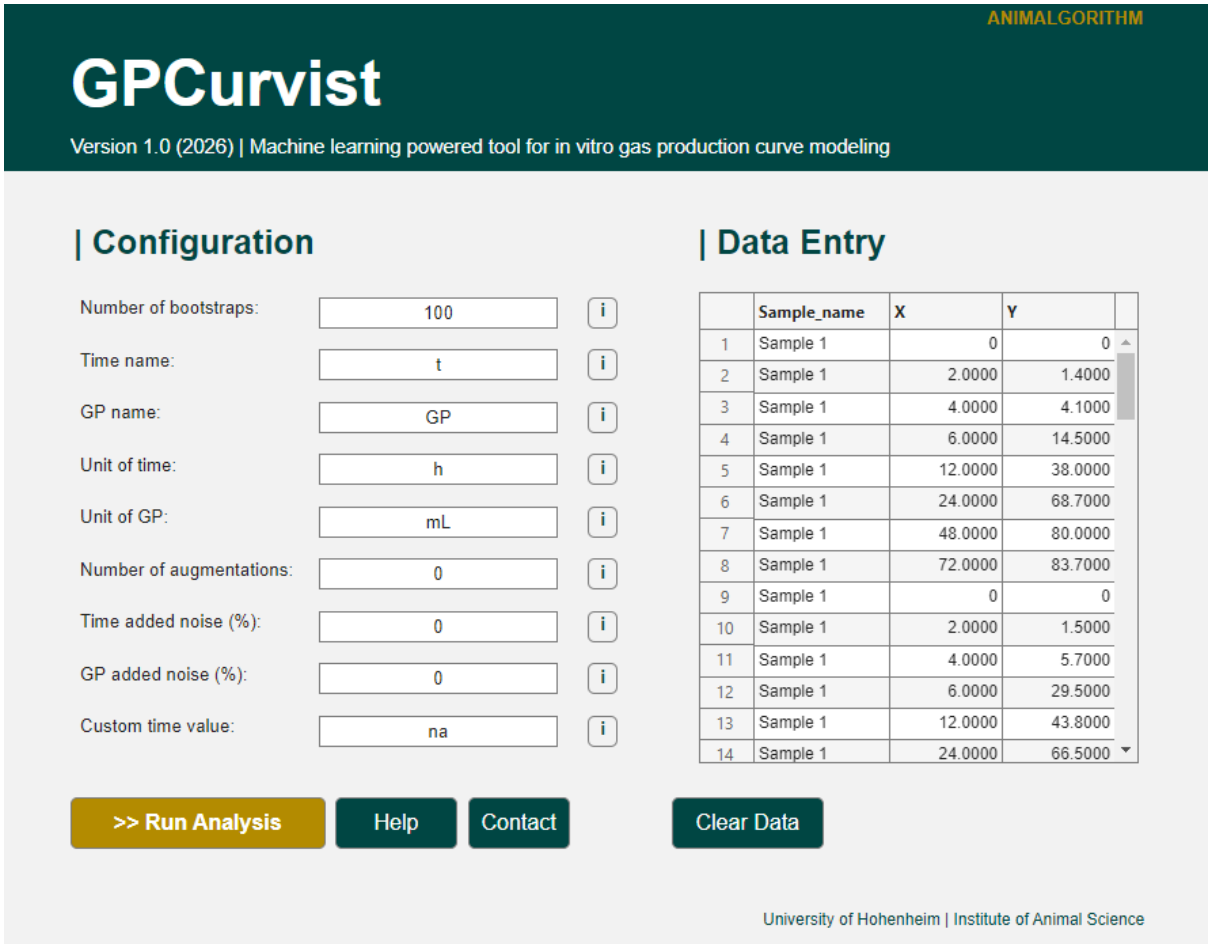

Figure 1. User interface of the GPCurvist

Below is a description of each input field, what it means, what to enter, and how it is validated.

1. Number of Bootstraps
   • **What to enter**: A positive integer ≥ 10 (e.g., 100, 200)
   • **Meaning**: Determines how many random resampled datasets are created to ensure robustness and uncertainty estimation.
   • **Validation**: Must be a whole number (integer); 10 or higher
2. Time name
   • **What to enter**: A text string (e.g., "t", "time", "time of incubation")
   • **Meaning**: The name of the TIME input variable; used as the X-axis label in plots.
   • **Validation**: Cannot be left empty

3. GP name
   • **What to enter**: A text string (e.g., "GP", "In vitro GP")
   • **Meaning**: Name of the GP variable; used as the Y-axis label in plots.
   • **Validation**: Cannot be left empty

4. Unit of time
   • **What to enter**: A text string (e.g., "h", "hour")
   • **Meaning**: The unit of measurement for the time; shown in axis labels.
   • **Validation**: Cannot be left empty

5. Unit of GP
   • **What to enter**: A text string (e.g., "liter", "L", "mL")
   • **Meaning**: Unit for the GP variable.
   • **Validation**: Cannot be left empty

6. Number of augmentations
   • **What to enter**: A non-negative integer (e.g., 0, 10, 50)
   • **Meaning**: Number of extra synthetic data points to generate using noise-added copies of your original data. Useful when working with limited datasets to improve model robustness. Set to 0 if you have sufficient data.
   • **Validation**: Must be 0 or higher

7. Time added noise (%)
   • **What to enter**: A non-negative number (e.g., 0, 2, 5)
   • **Meaning**: Amount of random noise (as a % of each original time value) to be added to the time-values for augmentation. Only applies if augmentation > 0.
   • **Validation**: Must be a non-negative number. If Number of augmentations is 0, then this must also be 0

8. GP added noise (%)
   • **What to enter**: A non-negative number (e.g., 0, 5, 10)
   • **Meaning**: Amount of random noise (as a % of each original GP value) to be added to the GP-values for augmentation. Only applies if augmentation > 0.
   • **Validation**: Must be a non-negative number. If Number of augmentations is 0, then this must also be 0

9. Custom time value
   • **What to enter**: A non-negative number (e.g., 24) or the text 'na' to skip
   • **Meaning**: Allows scenario testing at a specific time value. When set, the model evaluates the GP at this time.
   • **Validation**: Must be a non-negative number or the text 'na'. If 'na' is entered, the analysis at a custom time level is skipped

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Results

Once GPCurvist finishes analyzing your data and modeling is complete, the software automatically generates a results window with the following items inside:

This window contains **4 sheets**:

1. **Metrics**
    - Includes metrics (e.g., R^2, RMSE, inflection time, time required to reach desirable GP, etc.) from the curve fitting process for each sample including their 95% confidence intervals.
2. **Equations**
    - Contains the final symbolic formulas (ANN-based) fitted for each dataset. These are useful for interpretation or further use.
3. **Coefficients**
    - Includes the estimated neural network parameters (weights and biases) for each sample:
    - Each parameter also includes its **95% confidence intervals**, based on bootstrapping.
4. **Data & predictions**

Figures: Plots and metrics comparison

→ A **save** option is included in all sheets and Figures.

Insight from Results

The basic model used in **GPCurvist** is a simple artificial neural network with **single artificial neuron** and a **tanh activation function**, designed to fit smooth and meaningful in the context of time–GP analysis (Figure 1 and Table 1).

Model Equation: The fitted model takes the following mathematical form:

$$GP = \mathbf{A}\, tanh(\mathbf{c}\, t + \mathbf{b}) + \mathbf{B} \qquad \text{Equation 1}$$

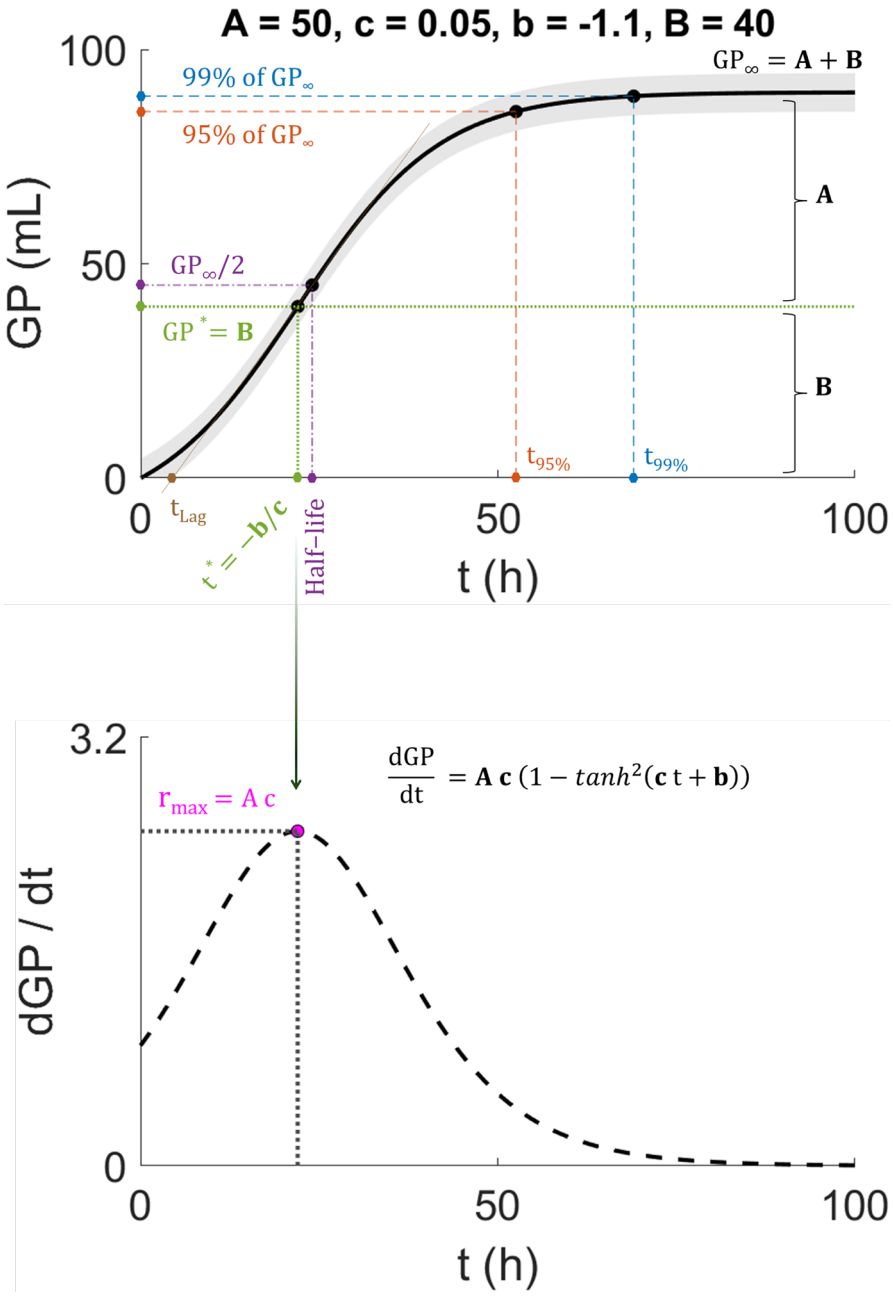

Figure 2: Schematic time–GP curve generated by the Equation 1, with parameters A = 50, c = 0.05, b = -1.1, and B = 40. For definitions see Table 1.

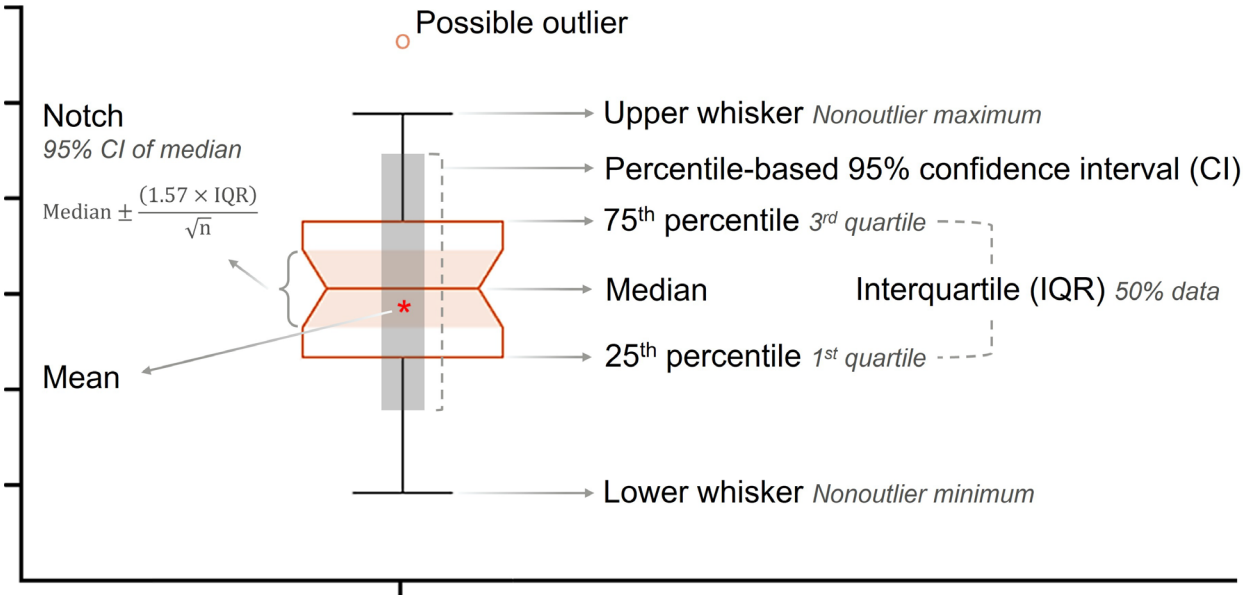

Figure 3. *Schematic representation of an enhanced box plot.*

The central box shows the interquartile range (IQR; 25th–75th percentile) with the median indicated by the horizontal line. Whiskers extend to the minimum and maximum non-outlier values, while possible outliers are plotted individually. The notch represents an approximate 95% confidence interval (CI) of the median, where non-overlapping notches suggest significant median differences between groups. In addition, the mean (red asterisk) and its bootstrap-derived 95% CI (grey rectangle) are displayed to provide the primary metric of interest, reflecting both central tendency and empirical uncertainty. While notches serve as a visual guide, all formal statistical inferences in this study are based on one-way ANOVA applied to the bootstrap distributions, followed by Tukey's honest significant difference (HSD) test for multiple comparison of means.

Table 1. Definition of GPCurvist model, parameters, and derived time–GP metrics.

	Explanation	**Equation**
Model	Time–GP curve describing how GP changes with time	$GP = A\ tanh(c\,t + b) + B$
First derivative	Rate of change of the GP with respect to time	$\frac{dGP}{dt} = A\,c\,(1 - tanh^2(c\,t + b))$
Parameters		
A	Amplitude of the curve determines how much the GP increases beyond the inflection point	
c	Steepness parameter: controls how quickly the GP changes as time increases	
b	Horizontal translation: shifts the curve left or right along the time axis	
B	GP at the inflection point; with B ≈ 0, the curve rises symmetrically from the origin toward the plateau	
Time–GP metrics		
r_{max}	Maximum slope of the curve; the steepest rate of increase in GP per unit time at the inflection point	$A\ c$
t^*	Time level at the inflection point, where GP changes most rapidly	$-\frac{b}{c}$
GP^*	GP value at the inflection point (i.e. t^*)	B
t_{Lag}	Lowest time value where a meaningful GP begins (GP_{min} = model-predicted GP at lowest time)	$t^* - \frac{GP^* - GP_{min}}{r_m}$
$Half-life$	Time at which 50% of the asymptotic GP is reached	$\frac{arctanh\left(0.5 - 0.5\frac{B}{A}\right) - b}{c}$
GP_∞	Asymptotic GP as time increases indefinitely	$A + B$
$t_{95\%}$	Time needed to achieve 95% of the GP_∞	$\frac{arctanh\left(0.95 - 0.05\frac{B}{A}\right) - b}{c}$
$t_{99\%}$	Time needed to achieve 99% of the GP_∞	$\frac{arctanh\left(0.99 - 0.01\frac{B}{A}\right) - b}{c}$