

DiagAccU

A Software Program for Uncertainty Estimation of Diagnostic Accuracy Measures under Parametric Distributions

Interface Documentation

v. 1.0.0

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1. Introduction

We developed a specialized computational framework for the unified estimation of uncertainty in diagnostic accuracy measures, to assist medical professionals and researchers in diagnostics. This framework has been implemented in the program *DiagAccU*. The program estimates and plots sixteen diagnostic threshold based diagnostic accuracy measures: sensitivity (Se), specificity (Sp), overall diagnostic accuracy (ODA), positive predictive value (PPV), negative predictive value (NPV), diagnostic odds ratio (DOR), likelihood ratio for a positive result (LR^+), likelihood ratio for a negative result (LR^-), Youden's index (JS), Euclidean distance (ED), concordance probability (CZ), Fowlkes–Mallows index (FMI), Cohen's kappa coefficient ($C\kappa$), prevalence-adjusted bias-adjusted Kappa ($PABAK$), F1 score ($F1S$), and Matthews correlation coefficient (MCC).

By utilizing the principles of uncertainty propagation, the program allows for the estimation and plotting of the sampling, measurement, and combined uncertainty of these measures, as well as the associated confidence intervals.

2. System Requirements

2.1. Processor

Intel Core i9® or equivalent CPU

2.2. System Memory (RAM)

32 GB+ recommended

2.3. Operating Systems

Microsoft Windows, Linux, Apple MacOs and iOS

2.4. Software Requirements

Wolfram Player®, freely available at [Wolfram Player](https://www.wolfram.com/player/) or Wolfram Mathematica®.

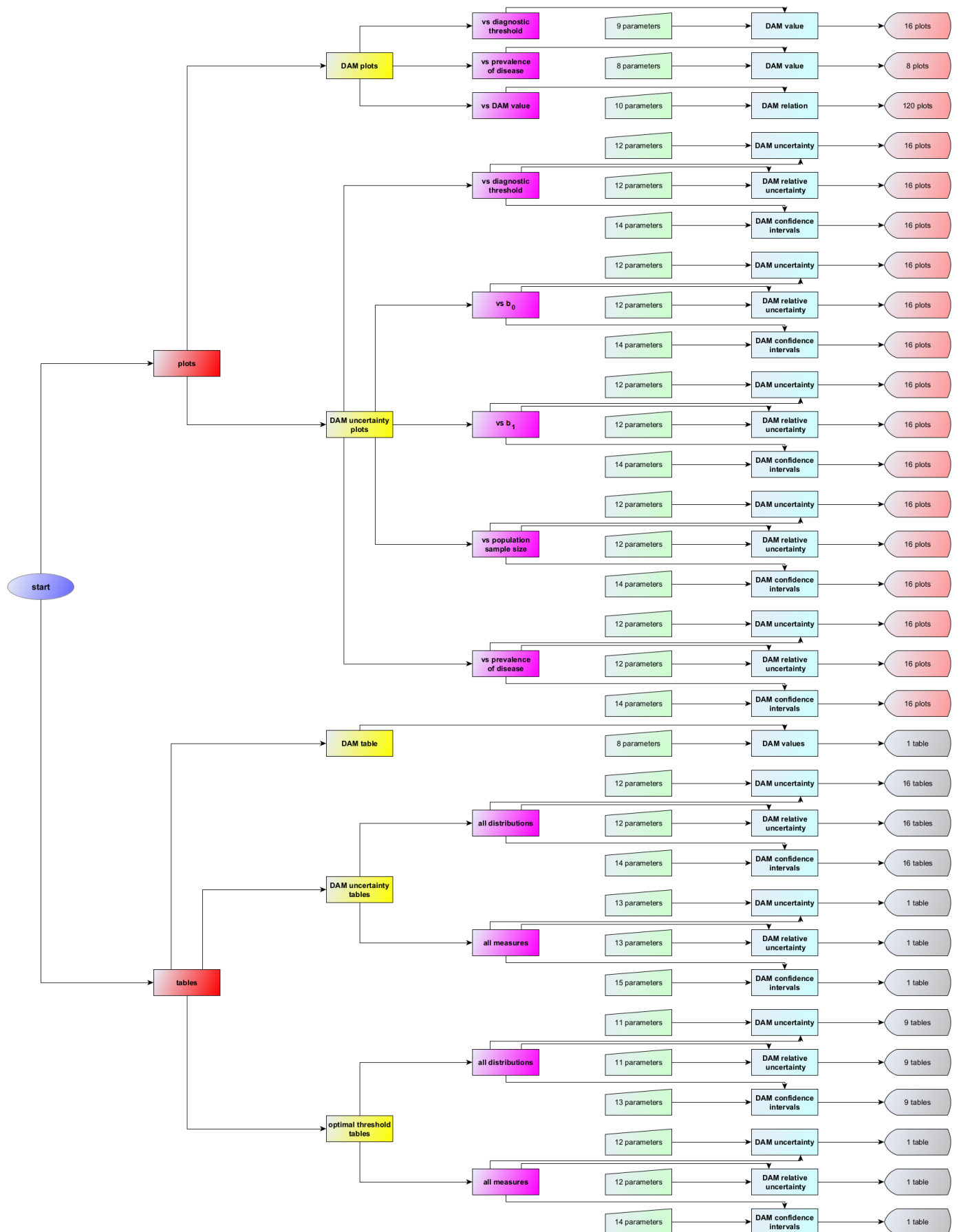


Figure 1. A simplified interface flowchart of the program *DiagAccU*.

3. Interface Overview

A simplified interface flowchart and a screenshot of the program *DiagAccU* are presented in Figures 1 and 2.

3.1. Tabbed Navigation

The program features an intuitive tabbed interface designed to streamline user interaction and facilitate effortless navigation across multiple modules and sub-modules. Each tab is clearly labeled to correspond with its respective module, allowing quick access to various functionalities.

3.2. Numerical Settings: Sliders

The program offers controls for numerical settings, which can be adjusted through sliders. Press the ‘alt’ or ‘opt’ key while dragging the mouse for more precise control. For even finer adjustments, also press the ‘shift’ or ‘ctrl’ keys.

3.3. Non-Numerical Settings

Buttons control these settings. Each button is labeled clearly to indicate its function.

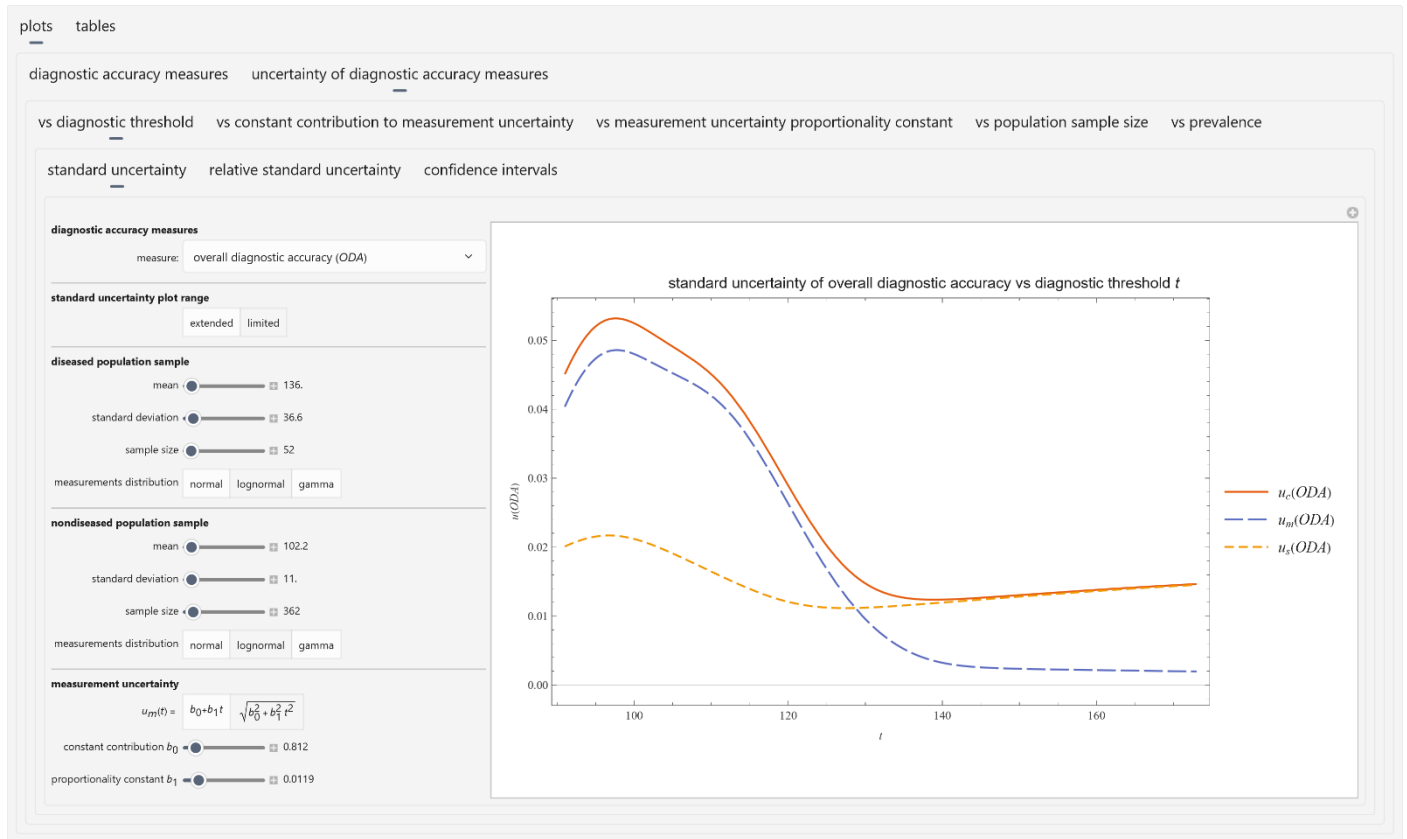


Figure 2. A screenshot of the program *DiagAccU*.

3.4. Additional Options

3.4.1. Plots

Users can select between an extended and limited plot range.

3.4.2. Tables

Users can define the number of decimal digits for results, ranging from 1 to 10.

4. Input variables and parameters

The program allows users to input a variety of variables and parameters, each with a specific range:

$$t: \text{maximum}(0, \text{minimum}(m_{\bar{D}} - 6s_{\bar{D}}, m_D - 6s_{\bar{D}})) - \text{maximum}(m_{\bar{D}} + 6s_{\bar{D}}, m_D + 6s_{\bar{D}})$$

$$n_D: 2 - 10,000$$

$$m_D: 0.1 - 10,000$$

$$s_D: 0.01 - 1,000$$

n_D : 2 – 10,000

m_D : 0.1 – 10,000

s_D : 0.01 – 1,000

v : 0.001 – 0.999

n_U : 20 – 10,000

b_0 : 0 – s_D

b_1 : 0 – 0.1000

p : 0.900 – 0.999

t, m_D, s_D, m_D , and s_D are defined in arbitrary units.

5. Modules and Submodules

The program is organized into two primary modules, each with multiple submodules:

5.1. Plots

5.1.1. Diagnostic Measures Plots

5.1.1.1. Plots:

- a) Sensitivity (Se),
- b) Specificity (Sp),
- c) Overall diagnostic accuracy (ODA),
- d) Positive predictive value (PPV),
- e) Negative predictive value (NPV),
- f) Diagnostic odds ratio (DOR),
- g) Likelihood ratio for a positive test result (LR^+),
- h) Likelihood ratio for a negative test result (LR^-),
- i) Youden's index (JS),
- j) Euclidean distance (ED),
- k) Concordance probability (CZ),
- l) Fowlkes–Mallows Index (FMI),
- m) Cohen's kappa coefficient ($C\kappa$),
- n) Prevalence-Adjusted Bias-Adjusted Kappa ($PABAK$),
- o) F1 Score ($F1S$),
- p) Matthews Correlation Coefficient (MCC),

versus:

- a) Diagnostic threshold t
- b) Each of the above measures.

5.1.1.2. Plots:

- a) Overall diagnostic accuracy (ODA),
- b) Positive predictive value (PPV),
- c) Negative predictive value (NPV),
- d) Youden's index (JS),
- e) Euclidean distance (ED),
- f) Concordance probability (CZ),
- g) Fowlkes–Mallows Index (FMI),
- h) Cohen's kappa coefficient ($C\kappa$),
- i) Prevalence-Adjusted Bias-Adjusted Kappa ($PABAK$),
- j) F1 Score ($F1S$),
- k) Matthews Correlation Coefficient (MCC),

versus prevalence or prior probability for disease v .

5.1.2. Standard Uncertainty Plots:

5.1.2.1. Plots:

- a) The standard sampling, measurement, and combined uncertainty
- b) The relative standard sampling, measurement, and combined uncertainty
- c) The associated confidence intervals

of the measures of the section 5.1.1.1, versus:

- a) The diagnostic threshold t
- b) The constant contribution b_0 to measurement uncertainty
- c) The measurement uncertainty proportionality constant b_1
- d) The total size of the population sample n
- e) The prevalence or prior probability for disease v

5.2. Tables

5.2.1. Diagnostic Measures Tables

For a diagnostic threshold t , the measures of the section 5.1.1.1 are tabulated.

5.2.2. Standard Uncertainty Tables:

The program tabulates the standard sampling, measurement, and combined uncertainty and relative uncertainty and the associated confidence intervals of the measures of the section 5.1.1.1 for a user-defined diagnostic threshold t and all the possible combinations of the distributions.

5.2.3. Optimal Threshold Tables:

The program estimates the diagnostic threshold that maximizes:

- a) Overall diagnostic accuracy (ODA),
- b) Youden's index (JS),
- c) Concordance probability (CZ),
- d) Fowlkes-Mallows Index (FMI),
- e) Cohen's kappa coefficient ($C\kappa$),
- f) Prevalence-adjusted bias-adjusted kappa ($PABAK$),
- g) F1 Score ($F1S$),
- h) Matthews Correlation Coefficient (MCC),

or minimizes Euclidean distance (ED), and tabulates the respective standard sampling, measurement, and combined uncertainty and relative uncertainty and the associated confidence intervals.

The diagnostic measures plots and tables modules allow the user to define:

- a) The mean and standard deviation of a diseased and a nondiseased population sample.
- b) The univariate distribution of each population (normal, lognormal, gamma).
- c) The diagnostic threshold t .

All modules allow the user to define:

- a) The size, mean and standard deviation of a diseased and a nondiseased population sample.
- b) The prevalence or prior probability for disease v .
- c) The univariate distribution of each population (normal, lognormal, gamma).
- d) A linear [$u_m(t) \cong b_0 + b_1 t$] or nonlinear [$u_m(t) = \sqrt{b_0^2 + b_1^2 t^2}$] equation of the measurement uncertainty versus the diagnostic threshold t and the number of the quality control measurements used to derive it.
- e) The diagnostic threshold t .
- f) The confidence level p of confidence intervals.

6. Source

6.1. Programming language

Wolfram Language

6.2. File format

Wolfram Notebook

6.3.Availability

The updated source is available at: <https://www.hcsl.com/Tools/DiagnosticAccuracy/ DiagAccU.nb>.

6.4. License

The *DiagAccu* program is licensed under the [Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License](https://creativecommons.org/licenses/by-nc-sa/4.0/).

7. Notation and Abbreviations

7.1.Variables and Parameters

t : diagnostic threshold of a diagnostic test

n_D : size of diseased population sample

m_D : mean of diseased population sample

s_D : standard deviation of diseased population sample

$n_{\bar{D}}$: size of nondiseased population sample

$m_{\bar{D}}$: mean of nondiseased population sample

$s_{\bar{D}}$: standard deviation of nondiseased population sample

v : prevalence or prior probability for disease

n_U : number of quality control measurements

b_0 : constant contribution to measurement uncertainty

b_1 : measurement uncertainty proportionality constant

p : confidence level

7.2.Diagnostic Accuracy Measures

Se : Sensitivity

Sp : Specificity

ODA : overall diagnostic accuracy

PPV : positive predictive value

NPV : negative predictive value

DOR : diagnostic odds ratio

LR^+ : likelihood ratio for a positive result

LR^- : likelihood ratio for a negative result

JS : Youden's index

ED : Euclidean distance

CZ : concordance probability

FMI : Fowlkes–Mallows Index

$C\kappa$: Cohen's *kappa coefficient*

$PABAK$: Prevalence-Adjusted Bias-Adjusted Kappa

$F1S$: F1 Score

MCC : Matthews Correlation Coefficient

8. Conclusion

The *DiagAccu* program offers a robust and user-friendly interface for medical professionals and researchers to estimate the uncertainty of diagnostic accuracy measures. Its modular design and comprehensive output options make it a valuable medical statistics and diagnostics tool.

9. Permanent Citation:

Chatzimichail RA, Chatzimichail T., Hatjimihail AT. *DiagAccu: A Computational Framework for Uncertainty Estimation of Diagnostic Accuracy Measures under Parametric Distributions*. Interface Documentation. Drama: Hellenic Complex Systems Laboratory, 2025. Available at: <https://www.hcsl.com/Tools/DiagnosticAccuracy/>

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