Author Contributions Checklist Form

This form documents the artifacts associated with the article (i.e., the data and code supporting the computational findings) and describes how to reproduce the findings.

# Part 1: Data

This paper **does not** involve analysis of external data (i.e., no data are used or the only data are generated by the authors via simulation in their code).

I certify that the author(s) of the manuscript have legitimate access to and permission to use the data used in this manuscript.

## Abstract

This projects invovles a simulation study which mimics phase I clinical trials. The data includes simulated dose-toxicity rates for 10,000 scenarios under different settings.

## Availability

Data **are** publicly available

Data **cannot be made** publicly available

If the data are publicly available, see the *Publicly available data* section. Otherwise, see the *Non-publicly available dat*a section, below.

### Publicly available data

Data are available online at:

https://github.com/staceyfu1029/PoP-design/tree/main/JASA/skeleton\_list

Data are available as part of the paper’s supplementary material.

Data are publicly available by request, following the process described here:

Data are or will be made available through some other mechanism, described here:

### Non-publicly available data

Discussion of lack of publicly available data:

## Description

### File format(s)

CSV or other plain text:

Software-specific binary format (.Rda, Python pickle, etc.):

Standardized binary format (e.g., netCDF, HDF5, etc.):

Other (described here):

The dose-toxicity rates for 10,000 scenarios under different settings are provided in the “xlsx” files.

### Data dictionary

Provided by the authors in the following file(s):

Data file(s) is (are) self-describiing (e.g., netCDF files)

Available at the following URL:

https://github.com/staceyfu1029/PoP-design/blob/main/JASA/skeleton\_list/Read.me

### Additional information (optional)

# Part 2: Code

## Abstract

We provide codes that used to run the PoP, BOIN and Keyboard designs in our simulation study and the codes for visualizing the result in the GitHub repository.

## Description

### Code format(s)

Script files

R  Python  Matlab

Other:

Package

R  Python  MATLAB toolbox

Other:

Reproducible report

R Markdown  Jupyter notebook

Other:

Shell script

Other (described here):

### **Supporting software requirements**

Version of primary software used

R version 4.3.0

Libraries and dependencies used by the code

BOIN, Keyboard, readxl, ggridges, ggplot2, viridis, hrbrthemes, gtable, grid, writexl

### Supporting system/hardware requirements (optional)

### Parallelization used

No parallel code used

Multi-core parallelization on a single machine/node

Number of cores used:

Multi-machine/multi-node parallelization

Number of nodes and cores used:

### License

MIT License (default)

BSD

GPL v3.0

Creative Commons

Other (described here):

### Additional information (optional)

# Part 3: Reproducibility workflow

## Scope

The provided workflow reproduces:

Any numbers provided in text in the paper

The computational method(s) presented in the paper (i.e., code is provided that implements the method(s))

All tables and figures in the paper

Selected tables and figures in the paper, as explained and justified here:

The provided codes can reproduce Figure 3, 4 and Table 2, 3 in the paper. Figure 1 and 2 are for illustration purpose and involve no data. Table 1 shows the decision boundaries that can be obtained using the function get\_boundary from R package PoPdesign.”

## Workflow details

### Location

The workflow is available:

As part of the paper’s supplementary material

In this Git repository: https://github.com/staceyfu1029/PoP-design/tree/main/JASA

Other:

### Format(s)

Single master code file

Wrapper (shell) script(s)

Self-contained R Markdown file, Jupyter notebook, or other literate programming approach

Text file (e.g., a readme-style file) that documents workflow

Makefile

Other (more detail in 'Instructions' below)

### Instructions

1. For Figure 3&4 or Table 2:

Step 1: simulate toxicity profiles

input the target toxicity phi and number of dose K in the code Skeleton\_list.R. 10,000 scenarios will be generated.

Step 2: run simulations and save the output

run simulations for the simulated toxicity profiles. PoP, BOIN, Keyboard, and CRM designs can implemented using the corresponding codes that are provided in this GitHub repositories (PoP.R, BOIN. R, Keyboard.R, and CRM.R). R workspaces should be saved after running those R scripts to generate the figures and tables.

Step 3: generate figures and tables

with the outputs from step 2 for different simulation settings mentioned in the paper, table 2 can generated using the R script Table2.R. Figure 3 and 4 can be generated using the R script Figure3&4.R.

2. For Table 3:

Table 3 can be generated using the R script Table3.R

Expected run-time

Approximate time needed to reproduce the analyses on a standard desktop machine:

<1 minute

1-10 minutes

10-60 minutes

1-8 hours

>8 hours

Not feasible to run on a desktop machine, as described here:

### Additional documentation (optional)

# Notes (optional)