SMART-MC (including MSCOR) Reproducibility Instructions

- We describe the reproducibility instructions for generating the tables and figures included in the main paper. Please refer to the following list to see which section describes the reproducibility of the tables and figures of the main paper, detailed as follows.
- Note that, real data is not shared on Github to comply with data sharing policy. To implement SMART-MC on another dataset, see Demo section.

Figures

- Figure 1: refer to SMART-MC Real Data Analysis.
- Figure 2: NA (concept diagram).
- Figure 3: NA (concept diagram).
- Figure 4: NA (concept diagram).
- Figure 5, 6: refer to SMART-MC Real Data Analysis.
- Other figures: S1, S2.

Tables

- Table 1: refer to MSCOR benchmark study.
- Other Tables: S1–S7.

DEMO

- This section demonstrates examples on practical implementations of MSCOR (for Black-box optimization purpose only, unrelated to SMART-MC implementation) and SMART-MC (backed by MSCOR; for synthetic data analysis).

1. Benchmark study

1. Go to MSCOR benchmark folder, run MSCOR_Benchmark_comparison.m, setting $(B, M) = (5, 5), (10, 20), (100, 5)$. The variable M represents n_b in the main paper.

2. To summarize the findings run MSCOR_post_evaluation.m. This yields results reported in Table 1 of the main paper (also **Table S1** and **Figure S1** in the supplementary material).

2. Simulation study

1. Go to Simulation Study folder, run SMART_MC_SIMULATION_STUDY_v2.m (for proposed method) and SMART_MC_SIMULATION_STUDY_NaiveMethod.m (for naive method to compare). Corresponding outputs are reported in **Table S2** of the supplementary material.

2. Go to Simulation Study / Simulation_Study_Non-gaussian folder, run SMART_MC_SIMULATION_STUDY_NonNormal.m (for proposed method) and SMART_MC_SIMULATION_STUDY_NonNormal_NaiveMethod.m (for naive method to compare). Corresponding outputs are reported in **Table S3** of the supplementary material.

3. Within Simulation Study folder, run SMART_MC_SIMULATION_MAD_sequence.m for MAD analysis reported in the paper. Corresponding outputs are reported in **Table S4** of the supplementary material.

4. Within Simulation Study folder, run SMART_MC_SIMULATION_parallel_v_single.m. This yields results reported in **Table S5** of the supplementary material.

3. Real data analysis

Note that the real data is not shared on Github respecting the data sharing policy, but only with journal editors (after de-identification).

1. Go to Real Data Analysis / Real Data folder, run collapsing_into_7_cats.R which converts the dataset with original 10 treatment categories, into considered 7 treatment categories.

2. In Real Data Analysis / Real Data folder, run exploratory_analysis.R, which generates Figure 1(a), 1(b).

3. Go to Real Data Analysis folder, run SMART_MC_Real_data.m. This yields all the source files required for results and **Figure S2** and **Table S6**.

4. Go to Real Data Analysis folder, run SMART_MC_p_values.R. This yields results noted in **Table S7**.

5. Within Real Data Analysis folder, run SMART_MC_Var_effect_plot.R which generates Figures 5,6(a).

6. Within Real Data Analysis folder, run SMART_MC_ODDS_ratio_calculation.m followed by SMART_MC_Odds_ratio_plot.R. This yields Figure 6(b).

4. DEMO

1. Go to DEMO / MSCOR demo folder. MSCOR_DEMO.m demonstrates a practical example of minimizing a non-convex function (namely, modified Ackley's function; see SMART-MC supplementary information for its exact form) using MSCOR.

2. Go to DEMO / SMART-MC demo folder. SMART_MC_DEMO.m demonstrates a practical example of SMART-MC estimation, backed with MSCOR, based on a dummy dataset.