User Manual for PCATS

June 25, 2023

Example 1. Step-by-step instruction of calling PCATS using a simple example of a binary treatment

This simple example provides step-by-step instructions on the use of the PCATS for estimating ATE and PrTE for the non-adaptive treatment setting. The example data are simulated from

- $X \sim N(0,1)$
- $A|X \sim Bernoulli(expit(-0.2 + 3X))$
- $Y|A, X \sim N(X + 5A, 1)$

For the non-adaptive treatment, staticGP function is used. With the continuous outcome Y in this simulation data, outcome type is set to "Continuous". tr.type gives the type of the treatment. In this example, the treatment A is a binary indicator variable, so tr.type is set to "Discrete". Since the example is not related to time, we create a "Time" variable with a fixed value 0 in the dataset. And time is set to "Time". Users do not need to specify time value for the case. The parameter x.explanatory specifies the prognostic variables W and x.confounding specifies the confounders V. The categorical variables in W and V should be specified in x.categorical. Users can define a link function by outcome.link whose default value is "identity". We use the default settings for the number of burn-in MCMC samples (burn.num) and the number of MCMC samples after burn-in (mcmc.num), which are 500 for both parameters. By default, estimates of averaged treatment effect and potential outcomes are reported. Users can also request PrTE for one or a list of supplied number(s) specified by c.margin. In the example, we set c.margin to "0,1,2" to print the corresponding treatment effect $PrTE_0$, $PrTE_1$ and $PrTE_2$, separately. For a continuous outcome, users can choose either GP or BART. For a binary outcome, only BART method is currently available.

```
library(pcatsAPIclientR)
  download.file("https://github.com/pcats-api/pcats_api_examples
      /raw/main/data/example1.csv", destfile="example1.csv")
  jobid <- pcatsAPIclientR::staticGP(datafile="example1.csv",</pre>
                                       outcome = "Y",
                                       treatment="A"
                                       time="Time",
                                       x.explanatory="X",
9
                                       x.confounding="X",
                                       burn.num=500, mcmc.num=500,
11
                                       outcome.type="Continuous",
12
                                       method="GP",
                                       tr.type="Discrete",
14
                                       c.margin="0")
16
  cat(paste0("JobID: ",jobid,"\n"))
```

Listing 1: R code of Example 1 to start computation.

```
JobID: e2db813e-89a2-4a35-bfa3-d34b5b2b0d0d
```

Listing 2: Output of R code of Example 1.

To make a request from R, we may submit the R code in Listing 1. After submitting the request, the system-generated id will be assigned to the job. Users can extract the job id from the response of the function staticGP and use the following code to wait for the job completion. In this example, the job id is "e2db813e-89a2-4a35-bfa3-d34b5b2b0d0d". If the job has been successfully done, the function will return with status="Done".

```
status <- pcatsAPIclientR::wait_for_result(jobid)
```

Listing 3: R code of Example 1 to wait for job completion.

To retrieve a job status without waiting for the completion (i.e., polling), one may use the following code.

```
status <- pcatsAPIclientR::job_status(jobid)
Listing 4: R code of Example 1 to poll job status.
```

After the job is successfully completed, the analysis results can be extracted from the API response by using the code:

```
if (status=="Done") {
    cat(pcatsAPIclientR::printgp(jobid))
3 }
```

Listing 5: R code of Example 1 to print results.

2. Python code

For Example 1, the following code calls PCATS API from a Python shell.

```
import pcats_api_client as pcats_api
2 import requests
4 r = requests.get("https://github.com/pcats-api/
      pcats_api_examples/raw/main/data/example1.csv")
6 with open("example1.csv", 'wb') as f:
      f.write(r.content)
9 jobid=pcats_api.staticgp(datafile="example1.csv",
10
          outcome="Y",
          treatment="A"
11
          time="Time",
12
          x_{explanatory="X"},
          x_confounding="X",
14
          burn_num=500,
15
16
          mcmc_num=500,
          outcome_type="Continuous",
17
         method="GP",
          tr_type="Discrete",
19
          c_margin="0")
20
21
22 print("JobID: {}".format(jobid))
23
24 status=pcats_api.wait_for_result(jobid)
25
if status == "Done":
27
     print(pcats_api.printgp(jobid))
28 else:
print("Error")
```

Listing 6: Python code of Example 1.

```
Average treatment effect:
   Contrast Estimation SD
                                LB
                                       UB PrTE(c=0)
  A = 0 - A = 1
                -5.048 0.198 -5.415 -4.662
 Potential outcomes:
5
                       LB
  A Estimation SD
6
       -0.122 0.089 -0.296 0.052
         4.926 0.112 4.708 5.140
9
  Plot URL: https://pcats.research.cchmc.org/api/job/e2db813e-89a2
     -4a35-bfa3-d34b5b2b0d0d/plot
  Plot Potential URL: https://pcats.research.cchmc.org/api/job/
     e2db813e-89a2-4a35-bfa3-d34b5b2b0d0d/plot/Potential
```

Listing 7: GP result output of Example 1.

The output in Listing 7 presents the result of causal treatment effect estimation. The average treatment effects are generated based on the user-specified treatment values. If the treatment variable is a factor, the sample potential outcomes for each level of the treatment variable are given. The pairwise comparisons of the treatment effects for all treatment groups are calculated. The first table shows the estimated ATE with standard deviation (SD) and the 95%

credible interval. The estimate of ATE is -5.05 with the corresponding 95% equal tail credible interval (CI) of (-5.42, -4.66), where the simulation true ATE is -5. And PrTE for c.margin=0 is provided in the column of PrTE(c=0). The second table presents the estimated average potential outcomes by treatment groups. It reports that the expected mean and its standard deviation for the potential outcomes are -0.12 and 0.09 for A=0 and 4.93 and 0.11 for A=1. The PCATS also provides several interactive figures. Users can access these figures by using Firefox, Microsoft Edge, Chrome, or Safari. Currently, Internet Explorer does not support these figures. The histograms of MCMC posterior estimates of ATE (Figure 1) and the average of the estimated potential outcomes (Figure 2) are presented in the URLs, which could be copied from Listing 7. The figures are interactive. By hovering the pointers, users are provided with the corresponding posterior estimates of the average treatment effect and potential outcomes. Users can hide any traces in the plot by clicking on the legend on the right side. In each histogram, users could obtain a more detailed report of the results by hovering the mouse over the specific histogram. For example, if a user is interested in finding if the probability of Y(0) - Y(1) is less than -5, then (s)he could click on the pink histogram as in Figure 1, then move the mouse to the bar at ATE = -5. The user could also save the entire figure into a PNG file which can be used for sharing the results.

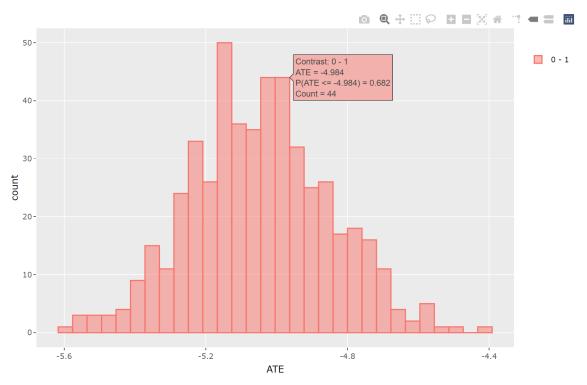


Figure 1: The histogram of the estimated average treatment effect

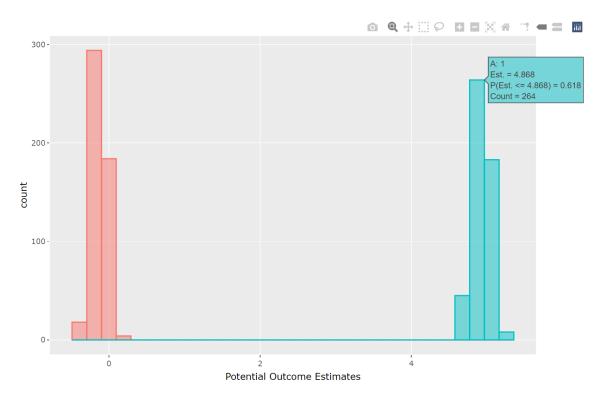


Figure 2: The histogram of the average of the estimated potential outcomes

Users could also set method to "BART" in the staticGP function. The BART results are shown in Listing 8. Comparing to Listing 7, we can see the results of GP and BART methods are quite similar in this case except GP provides more narrow confidence intervals in this example.

```
Average treatment effect:
    Contrast Estimation
                           SD
                                  LB
                                          UB PrTE(c=0)
   A = 0 - A = 1
                 -5.118 0.286 -5.743 -4.592
  Potential outcomes:
5
   A Estimation
                   SD
                           LB
                                 UB
6
         -0.166 0.166 -0.464 0.193
   0
7
          4.951 0.231 4.522 5.438
  Plot URL: https://pcats.research.cchmc.org/api/job/91a699dc-ed89
      -4213-beb3-1ea516f2292c/plot
12 Plot Potential URL: https://pcats.research.cchmc.org/api/job/91
      a699dc-ed89-4213-beb3-1ea516f2292c/plot/Potential
```

Listing 8: BART Result output of example 1

Example 2. Estimating CATE for a non-adaptive binary-continuous treatment

The PCATS can estimate the conditional average treatment effect (CATE) which captures heterogeneity of a treatment effect varying by treatment effect modifier(s). In this example, we consider a treatment variable A, and the treatment effect of A varies by gender. The data are generated as the following

- $X \sim N(0,1)$
- $Z \sim N(0,1)$
- Gender $\sim Bernoulli(0.5)$
- $A|X,Z \sim Bernoulli(expit(-0.2 + 3X))$
- $Y|A, X, Z, Gender \sim N(X + 5A + 3Z + 2A * Z + 2A * Gender, 1)$

In order to estimate CATE, users can specify the treatment effect modifier(s) with the treatment variable in tr.hte in the staticGP function. When specified, the corresponding interaction term(s) will be added into mean function of the PCATS model. In this example, by setting tr.hte ="Gender,Z", the interaction terms of Gender by treatment A and Z by treatment A are added into the mean function of the PCATS model.

For continuous treatment, PCATS calculates the sample potential outcomes based on the user-specified values of the variable which are given by tr.values. We request PCATS to report the treatment effects at the given values of the continuous treatment. The R code and Python example codes are provided as below.

```
1 library(pcatsAPIclientR)
  download.file("https://github.com/pcats-api/pcats_api_examples
      /raw/main/data/example2.csv", destfile="example2.csv")
  jobid <- pcatsAPIclientR::staticGP(datafile="example2.csv",</pre>
                                        outcome = "Y",
                                        treatment = "A".
                                        time="Time",
                                        x.explanatory="X,Z",
                                        x.confounding="X",
                                        tr.hte="Gender,Z"
                                        tr.type="Discrete",
12
                                        burn.num=500,
                                        mcmc.num=500,
14
                                        outcome.type="Continuous",
15
                                        method="GP",
16
                                        x.categorical="Gender")
17
19 status <- pcatsAPIclientR::wait_for_result(jobid)</pre>
```

```
if (status=="Done") {
   cat(pcatsAPIclientR::printgp(jobid))
  }
}
```

Listing 9: R code of Example 2.

The conditional average treatment effects of the sample data are estimated for the user-specified treatment sub-groups. control.tr defines the reference group and treat.tr defines the treatment group compared to the reference group. Then, the estimated CATE and PrCTE and their 95% confidence intervals at each level of "Gender" will be reported.

Listing 10: R code of Example 2 – CATE.

```
import pcats_api_client as pcats_api
2 import requests
4 r = requests.get("https://github.com/pcats-api/pcats_api_
      examples/raw/main/data/example2.csv")
6 with open("example2.csv", 'wb') as f:
      f.write(r.content)
9 jobid=pcats_api.staticgp(datafile="example2.csv",
         outcome="Y",
10
          treatment="A",
11
          time="Time",
12
13
          x_explanatory="X,Z",
         x_confounding="X",
14
         tr_hte="Gender,Z",
15
         tr_type="Discrete",
16
17
          burn_num=500,
18
          mcmc_num=500,
         outcome_type="Continuous",
19
         method="GP",
         x_categorical="Gender")
21
23 print("JobID: {}".format(jobid))
status=pcats_api.wait_for_result(jobid)
26
if status == "Done":
```

```
print(pcats_api.printgp(jobid))
    print("Error")
30
      exit()
31
32
33 #CATE
34
jobid_cate=pcats_api.staticgp_cate(jobid=jobid,
         x="Gender",
          control_tr="1",
37
          treat_tr="0",
38
          c_margin="0")
39
40
41 print("CATE JobID: {}".format(jobid_cate))
42
43 status=pcats_api.wait_for_result(jobid_cate)
44
45 if status=="Done":
     print(pcats_api.printgp(jobid_cate))
47 else:
print("Error")
```

Listing 11: Python code of Example 2.

```
Average treatment effect:
   Contrast Estimation SD
                                 I.B
  A = 0 - A = 1
                -6.243 0.184 -6.611 -5.9
5 Potential outcomes:
   A Estimation
                 SD
                        LB
       0.014 0.095 -0.150 0.212
  0
         6.257 0.092 6.086 6.442
10 Plot URL: https://pcats.research.cchmc.org/api/job/1f47521c-427f
      -487a-a671-c4e95253d043/plot
12 Plot Potential URL: https://pcats.research.cchmc.org/api/job/1
    f47521c-427f-487a-a671-c4e95253d043/plot/Potential
```

Listing 12: Result output of Example 2.

Listing 13: Result output of Example 2 – CATE.

The output are presented in Listing 12. The first table shows the estimated ATE by the pairwise comparison for each level of the treatment. The second table presents the estimated potential outcomes for each level of the treatment. The table in Listing 13 shows the estimated CATEs of the user-specified treatment groups for each level of "Gender". In this example, the simulation true values

of the treatment effect of A given Z=0 were set as -5 for Gender= 0 and -7 for Gender= 1. The estimated PrCTEs for c.margin="0" by "Gender" group are shown in the last column. The interactive figures of the estimated CATEs in Figure 3 can be retrieved through the URL link shown at the bottom of the result in Listing 13. The violin plots show the kernel probability densities of the estimated CATEs, and the box plots show the medians of the estimated CATEs with the boxes indicating the interquartile ranges. The corresponding values are also shown in the hover text.

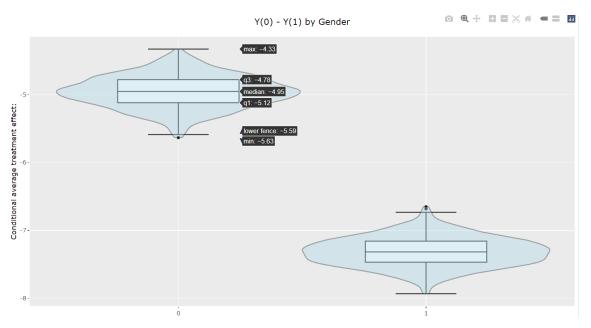


Figure 3: Estimates of the conditional average treatment effect by Gender

Example 3: Estimating ATE for adaptive binary treatment strategies

The dynamicGP function is designed to estimate the ATE for data with two time points. This example shows how to use the dynamicGP function. The simulation data were generated from the following simulation setting:

- $X \sim N(0,1)$
- $A_1 \sim Bernoulli(0.5)$
- $L_1|A_1, X \sim N(0.25 + 0.3A_1 0.2X, 1)$
- $A_2|L_1, A_1, X \sim Bernoulli(expit(-0.2 0.38A_1 + L_1))$

• $Y|A_1, X, L_1, A_2 \sim N(-2 + 2.5A_1 + 3.5A_2 + 0.5A_1A_2 - 0.6L_1, sd = 2)$

The expectation of the potential outcomes $Y_i(a_1, a_2)$ can be derived as $E(Y(a_1, a_2)) = -2.15 + 2.32a_1 + 3.5a_2 + 0.5a_1a_2$. The R code and Python code are shown below:

1. R code

```
library(pcatsAPIclientR)
download.file("https://github.com/pcats-api/pcats_api_examples
      /raw/main/data/example3.csv", destfile="example3.csv")
5 jobid <- pcatsAPIclientR::dynamicGP(datafile="example3.csv",</pre>
                                        stg1.outcome="L1",
                                        stg1.treatment="A1"
                                        stg1.time="Time1",
                                        stg1.x.explanatory="X",
                                        stg1.x.confounding="X",
                                        stg1.outcome.type="
      Continuous",
                                        stg2.outcome="Y",
12
                                        stg2.treatment="A2",
13
                                        stg2.time="Time2",
14
                                        stg2.x.explanatory="X,L1",
15
                                        stg2.x.confounding="X,L1",
16
                                        stg2.outcome.type="
17
      Continuous",
                                        burn.num=500,
18
                                        mcmc.num=500,
19
                                        stg1.tr.type="Discrete",
20
                                        stg2.tr.type="Discrete",
21
                                        method="GP")
22
23
24 status <- pcatsAPIclientR::wait_for_result(jobid)</pre>
if (status=="Done") {
27
  cat(pcatsAPIclientR::printgp(jobid))
```

Listing 14: R code of Example 3.

```
stg1_outcome_type="Continuous",
           stg2_outcome="Y'
16
           stg2_treatment="A2".
17
           stg2_time="Time2",
18
           stg2_x_explanatory="X,L1",
19
           stg2_x_confounding="X,L1",
20
21
           stg2_outcome_type="Continuous",
           burn_num=500,
22
           mcmc_num=500,
           stg1_tr_type="Discrete",
24
           stg2_tr_type="Discrete",
25
           method="GP")
26
27
28 print("JobID: {}".format(jobid))
29
30 status=pcats_api.wait_for_result(jobid)
31
32 if status=="Done":
      print(pcats_api.printgp(jobid))
33
34 else:
print("Error")
```

Listing 15: Python code of Example 3.

The results of GP and BART methods are shown in Listings 16 and 17. Both methods provide similar estimates. The statistical results of ATE and potential outcomes at two time points are shown in the output tables. Stage 1 shows the results of the first time point and Stage 2 shows the second time point. For Stage 1, the interpretation of the result is similar to that in non-adaptive treatment. For Stage 2, the ATE is the total effect. For example, the first row of ATEs given in Listing 16 is an estimate for $E(Y(a_1=0,a_2=0))-E(Y(a_1=0,a_2=1))$. The estimated ATE of -3.8 is closed to the simulation true value of -3.5 and the 95% credible interval, (-4.64, -2.82), covers the true value, as displayed in the histogram of Figure 4. The estimated potential outcomes are also accurate and its histogram is shown in Figure 5.

```
1 Stage 1:
2 Average treatment effect:
                             SD
                                    I.B
                                            UB
      Contrast Estimation
   A1=0 - A1=1
                  -0.435 0.149 -0.743 -0.162
6 Potential outcomes:
                   SD
   A1 Estimation
                           LB
           0.068 0.083 -0.106 0.220
    0
           0.502 0.070 0.365 0.637
9
11 Stage 2:
12 Average treatment effect:
13
                   Contrast Estimation
                                           SD
                                                  LB
                                                          UB
   A1=1 & A2=1 - A1=0 & A2=1
                                  3.106 0.472
                                                2.153
                                                       3.985
14
   A1=1 & A2=1 - A1=0 & A2=0
                                  6.893 0.421
                                                6.075
                                                       7.640
  A1=1 & A2=1 - A1=1 & A2=0
                                  4.191 0.427
                                               3.290
                                                      4.976
16
17 A1=0 & A2=1 - A1=0 & A2=0
                                  3.787 0.468 2.821
                                                      4.635
                                  1.085 0.523 0.127 2.064
  A1=0 & A2=1 - A1=1 & A2=0
18
   A1=0 & A2=0 - A1=1 & A2=0
                                  -2.702 0.428 -3.494 -1.849
```

```
20
  Potential outcomes:
                       SD
                                     UB
   A1 A2 Estimation
                              LB
              4.467 0.228 4.043
                                 4.937
              1.360 0.358 0.625 2.035
    0 1
24
    0
       0
             -2.426 0.279 -2.915 -1.826
25
              0.276 0.285 -0.323 0.795
26
    1
      0
27
28 Plot URL: https://pcats.research.cchmc.org/api/job/3bf0e733-a381
      -4525-9a5a-5c8552b634e2/plot
29
30 Plot Potential URL: https://pcats.research.cchmc.org/api/job/3
   bf0e733-a381-4525-9a5a-5c8552b634e2/plot/Potential
```

Listing 16: GP result output of Example 3.

```
1 Stage 1:
2 Average treatment effect:
     Contrast Estimation SD
                                   LB
   A1=0 - A1=1
                    -0.449 0.17 -0.767 -0.115
6 Potential outcomes:
   A1 Estimation SD
                            LB
           0.053 0.118 -0.151 0.277
   0
9
           0.502 0.117 0.282 0.736
10
11 Stage 2:
{\tt 12} Average treatment effect:
                     Contrast Estimation
                                             SD
13
  A1=1 & A2=1 - A1=0 & A2=1
                               3.107 0.530 2.063 4.110
                                   6.585 0.546 5.501 7.692
4.207 0.519 3.136 5.232
   A1=1 & A2=1 - A1=0 & A2=0
15
   A1=1 & A2=1 - A1=1 & A2=0
16
   A1=0 & A2=1 - A1=0 & A2=0
                                   3.477 0.578 2.281 4.532
17
   A1=0 & A2=1 - A1=1 & A2=0
                                   1.099 0.612 -0.080 2.305
18
   A1=0 & A2=0 - A1=1 & A2=0
                                  -2.378 0.542 -3.421 -1.321
20
21 Potential outcomes:
                       SD
  A1 A2 Estimation
                               LB
22
    1 1
               4.389 0.354 3.652 5.076
    0 1
              1.282 0.445 0.424 2.165
24
              -2.196 0.407 -3.014 -1.416
0.182 0.422 -0.683 1.016
25
    0
       0
26
28 Plot URL: https://pcats.research.cchmc.org/api/job/5f0e0df5-8d0b-4
      c15-91d2-b2e0d8f193e8/plot
30 Plot Potential URL: https://pcats.research.cchmc.org/api/job/5
      f0e0df5-8d0b-4c15-91d2-b2e0d8f193e8/plot/Potential
```

Listing 17: BART result output of Example 3.

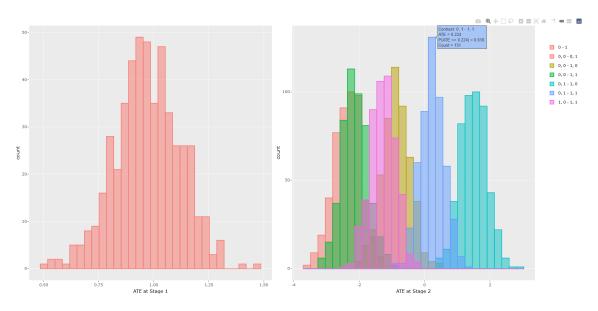


Figure 4: The histogram of the estimated average treatment effect at each stage.

Example 4: Estimating CATE for adaptive binary treatment strategies

This example presents users how to use the API to estimate the condition average treatment effect (CATE) for data with two time points. The simulation setting is as follows:

- $X \sim N(0,1)$
- $M \sim Bernoulli(0.4)$
- $A_1 \sim Bernoulli(expit(0.3 0.5X 0.4M))$
- $L_1|A_1, X, M \sim N(0.75X 0.75A_1 0.25A_1M + 0.5M, 1)$
- $A_2|L_1, A_1, X, M \sim Bernoulli(expit(0.5X + 0.2A_1 0.05L_1 0.1L_1A_1 0.01L_1^2 0.2M))$
- $Y|A_1, X, M, L_1, A_2 \sim N(3 + 0.5A_1 + 0.4A_2M L_1 L_1^2 + 2A_2 A_1A_2 + M, sd = 2)$

The R code and Python code are shown below:

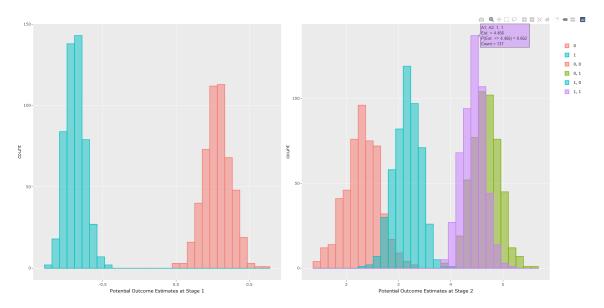


Figure 5: The histogram of the average of the estimated potential outcomes at each stage.

```
jobid <- pcatsAPIclientR::dynamicGP(datafile="example4.csv",</pre>
                                          stg1.outcome="L1",
                                          stg1.treatment="A1",
                                          stg1.time="Time1",
8
                                          stg1.x.explanatory="X,M",
9
                                          stg1.x.confounding="X,M",
                                          stg1.outcome.type="
11
      Continuous",
                                          stg1.tr.hte="M",
12
                                          stg1.tr.type="Discrete",
13
                                          stg2.outcome="Y",
14
                                          stg2.treatment="A2",
15
                                          stg2.time="Time2",
16
                                          stg2.x.explanatory="X,L1,M
17
18
                                          stg2.x.confounding="X,L1,M
                                          stg2.outcome.type="
19
      Continuous",
                                          stg2.tr2.hte="M",
20
                                          stg2.tr.type="Discrete",
21
                                         burn.num=500,
22
                                         mcmc.num=500,
23
                                         x.categorical = "M",
24
25
                                         method="GP")
27 status <- pcatsAPIclientR::wait_for_result(jobid)</pre>
28
29 if (status=="Done") {
```

```
cat(pcatsAPIclientR::printgp(jobid))
31 }
32
jobidcate <- pcatsAPIclientR::dynamicGP.cate(</pre>
  jobid=jobid,
34
   x="M",
35
    control.tr="0,0",
36
   treat.tr="1,0")
37
39 status <- pcatsAPIclientR::wait_for_result(jobidcate)</pre>
40
41 if (status=="Done") {
cat(pcatsAPIclientR::printgp(jobidcate))
43 }
```

Listing 18: R code of Example 4.

```
import pcats_api_client as pcats_api
2 import requests
4 r = requests.get("https://github.com/pcats-api/
      pcats_api_examples/raw/main/data/example4.csv")
6 with open("example4.csv", 'wb') as f:
      f.write(r.content)
9 jobid=pcats_api.dynamicgp(datafile="example4.csv",
          stg1_outcome="L1"
10
          stg1_treatment="A1",
11
          stg1_time="Time1",
          stg1_x_explanatory="X,M",
13
14
          stg1_x_confounding="X,M",
          stg1_outcome_type="Continuous",
15
         stg1_tr_hte="M",
16
         stg2_outcome="Y"
17
          stg2_treatment="A2",
18
19
          stg2_time="Time2",
         stg2_x_explanatory="X,L1,M",
20
21
         stg2_x_confounding="X,L1,M",
          stg2_outcome_type="Continuous",
22
          stg2_tr2_hte="M",
23
24
          burn_num=500,
         mcmc_num=500,
25
         stg1_tr_type="Discrete",
26
          stg2_tr_type="Discrete",
27
          x_categorical="M",
28
          method="GP")
29
print("JobID: {}".format(jobid))
status=pcats_api.wait_for_result(jobid)
34
35 if status=="Done":
     print(pcats_api.printgp(jobid))
37 else:
print("Error")
```

```
39 exit()
40
41 #CATE
42
43 jobid_cate=pcats_api.dynamicgp_cate(jobid=jobid,
          x = "M"
44
          control_tr="0,0",
45
          treat_tr="1,0")
46
48 print("CATE JobID: {}".format(jobid_cate))
49
50 status=pcats_api.wait_for_result(jobid_cate)
51
52 if status=="Done":
    print(pcats_api.printgp(jobid_cate))
53
54 else:
print("Error")
```

Listing 19: Python code of Example 4.

```
1 Stage 1:
2 Average treatment effect:
      Contrast Estimation
                                SD
                     0.971 0.149 0.663 1.243
   A1 = 0 - A1 = 1
6 Potential outcomes:
7 A1 Estimation SD
                              LB
            0.284 0.091 0.115 0.466
    0
8
            -0.687 0.066 -0.817 -0.558
9
    1
11 Stage 2:
Average treatment effect:
                       Contrast Estimation
                                                SD
                                                        LB
   A1=1 & A2=0 - A1=0 & A2=0
                                  0.851 0.439 0.046 1.736
14
15 A1=1 & A2=0 - A1=1 & A2=1
                                     -1.271 0.383 -2.045 -0.555
   A1=1 & A2=0 - A1=0 & A2=1
                                     -1.494 0.405 -2.280 -0.756
   A1=0 & A2=0 - A1=1 & A2=1
A1=0 & A2=0 - A1=0 & A2=1
                                     -2.122 0.400 -2.935 -1.316
17
                                     -2.346 0.453 -3.187 -1.380
   A1=1 & A2=1 - A1=0 & A2=1
                                     -0.224 0.392 -0.918 0.594
19
20
21 Potential outcomes:
22 A1 A2 Estimation
                         SD
                                LB
                                       UB
       0
                3.164 0.250 2.705 3.661
23
                2.313 0.334 1.650 2.957
    0 0
24
                4.435 0.213 4.040 4.852
25
                4.659 0.282 4.131 5.250
    0 1
26
27
28 Plot URL: https://pcats.research.cchmc.org/api/job/f6eb3598-95c1-4
       a4c-8696-70b6e24042d5/plot
30 Plot Potential URL: https://pcats.research.cchmc.org/api/job/
       f6eb3598-95c1-4a4c-8696-70b6e24042d5/plot/Potential
32 Conditional average treatment effect:
                      Constrast M Estimation
                                                  SD
                                                          LB

      34
      A1=1 & A2=0 - A1=0 & A2=0 0
      0.599 0.449 -0.295 1.439

      35
      A1=1 & A2=0 - A1=0 & A2=0 1
      1.179 0.479 0.358 2.200
```

```
36
37 Plot URL: https://pcats.research.cchmc.org/api/job/ca4bf80a-482c-47
f1-afa9-6e8d2977b6d9/plot
```

Listing 20: Result output of Example 4.

At Stage 1, the simulation true value of the sample ATE is 0.86, the true stage-2 sample ATEs of Y(0,0)-Y(0,1), Y(0,0)-Y(1,0, Y(0,0)-Y(1,1), Y(0,1)-Y(1,0), Y(0,1)-Y(1,1), and <math>Y(1,0)-Y(1,1) are about -2.17, -1.03, -2.20, 1.14, -0.03, and -1.17 respectively. The 95% credible intervals correctly cover the true expected potential outcomes.

By the simulation design, the true sample CATEs of (Y(1,0) - Y(0,0)|M=0) and (Y(1,0) - Y(0,0)|M=1) are 0.68 and 1.49. The last table shows the estimated CATE for each level of M, and all 95% credible intervals cover the true values.

Example 5: Binary outcome at stage 1 and continuous outcome at stage 2

This example shows how to use the API to estimate ATE for data with two different types of outcome at time points. Since the intermediate outcome L_1 is binary, a BART method is used for this example.

- $U_0 \sim Bernoulli(0.4)$
- $A_1 \sim Bernoulli(0.5)$
- $L_1|A_1, U_0 \sim Bernoulli(expit(0.25 + 0.3A_1 0.2U_0 0.05A_1U_0))$
- $A_2|L_1, A_1, U_0 \sim Bernoulli(expit(0.4 + 0.5A_1 0.3L_1 0.4A_1L_1))$
- $Y|A_1, U_0, L_1, A_2 \sim N(2.5 0.5A_1 0.75A_2 + 0.2A_1A_2 U_0, sd = 0.2)$

The expectation of Y can be calculated by $E(Y(a_1, a_2)) = 2.1 - 0.5a_1 - 0.75a_2 + 0.2a_1a_2$. The R code and Python code are listed below:

```
stg2.outcome="Y",
14
                                          stg2.treatment="A2",
                                         stg2.time="Time2",
15
                                         stg2.x.explanatory="U0,L1"
16
                                         stg2.x.confounding="U0,L1"
17
                                         stg2.outcome.type="
18
       Continuous",
                                         stg2.tr.type="Discrete",
19
                                         burn.num=500,
20
                                         mcmc.num=500,
21
                                         method="BART")
22
23
24 status <- pcatsAPIclientR::wait_for_result(jobid)</pre>
26 if (status=="Done") {
   cat(pcatsAPIclientR::printgp(jobid))
27
```

Listing 21: R code of Example 5.

```
import pcats_api_client as pcats_api
2 import requests
4 r = requests.get("https://github.com/pcats-api/
      pcats_api_examples/raw/main/data/example5.csv")
6 with open("example5.csv", 'wb') as f:
      f.write(r.content)
9 jobid=pcats_api.dynamicgp(datafile="example5.csv",
          stg1_outcome="L1"
10
          stg1_treatment="A1",
11
          stg1_time="Time1",
12
          stg1_x_explanatory="U0",
13
14
          stg1_x_confounding="U0",
          stg1_outcome_type="Discrete",
15
16
          stg1_tr_type="Discrete",
          stg2_outcome="Y",
17
          stg2_treatment="A2",
18
19
          stg2_time="Time1",
          stg2_x_explanatory="U0,L1",
20
          stg2_x_confounding="U0,L1",
21
          stg2_outcome_type="Continuous",
22
23
          stg2_tr_type="Discrete",
24
          burn_num=500,
          mcmc_num=500,
25
          method="BART")
27
28 print("JobID: {}".format(jobid))
status=pcats_api.wait_for_result(jobid)
32 if status=="Done":
print(pcats_api.printgp(jobid))
```

```
else:
print("Error")
```

Listing 22: Python code of Example 5.

```
1 Stage 1:
2 Average treatment effect:
      Contrast Estimation
                             SD
                                  LB
                                        UB
                    0.064 0.05 -0.03 0.16
   A1 = 0 - A1 = 1
  Potential outcomes:
   A1 Estimation SD
                          I.B
           0.484 0.037 0.410 0.551
8
9
    1
            0.421 0.035 0.347 0.483
11 Stage 2:
12 Average treatment effect:
                    Contrast Estimation
                                            SD
                                                   LB
13
   A1=0 & A2=1 - A1=1 & A2=1 0.281 0.040 0.206
14
                                                       0.357
   A1=0 & A2=1 - A1=0 & A2=0
                                  -0.777 0.045 -0.864 -0.686
15
   A1=0 & A2=1 - A1=1 & A2=0
                                  -0.248 0.048 -0.337 -0.150
   A1=1 & A2=1 - A1=0 & A2=0
                                  -1.058 0.045 -1.141 -0.970
17
   A1=1 & A2=1 - A1=1 & A2=0
                                  -0.529 0.046 -0.621 -0.434
18
   A1=0 & A2=0 - A1=1 & A2=0
                                   0.529 0.049 0.436 0.630
19
21 Potential outcomes:
                       SD
                             LB
                                    UB
   A1 A2 Estimation
22
    0
              1.332 0.029 1.276 1.387
23
24
    1
       1
              1.051 0.029 1.003 1.110
              2.109 0.035 2.034 2.174
25
26
              1.580 0.038 1.507 1.651
27
  Plot URL: https://pcats.research.cchmc.org/api/job/eaa716cc-d14a
       -492f-b6fa-f0cdec3aa8d3/plot
30 Plot Potential URL: https://pcats.research.cchmc.org/api/job/
      eaa716cc-d14a-492f-b6fa-f0cdec3aa8d3/plot/Potential
```

Listing 23: Result output of Example 5.

The estimated results of E(Y(a1 = 0, a2 = 0)), E(Y(a1 = 0, a2 = 1)), E(Y(a1 = 1, a2 = 0)) and E(Y(a1 = 1, a2 = 1)) are 2.11, 1.33, 1.58 and 1.05, which are close to the true values 2.1, 1.35, 1.6 and 1.05.

Example 6. Estimating ATE for bounded data

The PCATS can handle the outcome bounded by the minimum and maximum limits by using the GP method. For this type of outcome, users need to set the option outcome.bound_censor as "bounded" and specify the lower and upper bounds in outcome.lb and outcome.ub. Because the original BART method cannot handle the bounded data, the PCATS will fit the data without considering the bounds if the BART method is chosen. This example is similar to Example 1 except that the outcome Y has the minimum value of zero. For comparison, results are generated using both GP and BART methods.

```
library(pcatsAPIclientR)
3 download.file("https://github.com/pcats-api/pcats_api_examples/raw/
      main/data/example6.csv", destfile="example6.csv")
5 #GP
6 jobid <- pcatsAPIclientR::staticGP(datafile="example6.csv",</pre>
                                        outcome="Y",
                                        treatment = "A",
                                        time="Time",
9
                                        x.explanatory="X",
10
                                        x.confounding="X",
11
                                        burn.num=500,
12
13
                                        mcmc.num=500,
                                        outcome.type="Continuous",
14
                                        method="GP",
15
                                        tr.type="Discrete",
16
                                        outcome.1b=0,
17
18
                                        outcome.ub="inf",
                                        outcome.bound_censor="bounded")
19
21 status <- pcatsAPIclientR::wait_for_result(jobid)</pre>
23 if (status=="Done") {
cat(pcatsAPIclientR::printgp(jobid))
25 }
26
27 #BART
jobid <- pcatsAPIclientR::staticGP(datafile="example6.csv",</pre>
                                        outcome="Y",
                                        treatment = "A",
                                        time="Time",
31
                                        x.explanatory="X",
32
                                       x.confounding="X",
33
                                        burn.num=500,
34
35
                                        mcmc.num=500,
                                        outcome.type="Continuous",
36
                                        method="BART")
38
39 status <- pcatsAPIclientR::wait_for_result(jobid)</pre>
40
41 if (status=="Done") {
42 cat(pcatsAPIclientR::printgp(jobid))
43 }
```

Listing 24: R code of Example 6.

```
Plot Potential URL: https://pcats.research.cchmc.org/api/job/1 f44596c-2940-4312-8118-91e174bae520/plot/Potential
```

Listing 25: GP result output of Example 6.

```
Average treatment effect:
    Contrast Estimation
                           SD
                                  LB
                                         UB
   A = 0 - A = 1
                -4.584 0.216 -5.003 -4.179
5 Potential outcomes:
   A Estimation
                 SD
                         LB
                               UB
6
          0.501 0.122 0.248 0.719
          5.085 0.168 4.741 5.395
  1
10 Plot URL: https://pcats.research.cchmc.org/api/job/db78434a-9842-4
      ef5-ad22-b43c5fee57ce/plot
12 Plot Potential URL: https://pcats.research.cchmc.org/api/job/
      db78434a-9842-4ef5-ad22-b43c5fee57ce/plot/Potential
```

Listing 26: BART result output of Example 6.

Listing 25 shows that the GP results in the posterior mean of -4.84 and the credible interval of (-5.14, -4.50), and Listing 26 shows that the BART results in the posterior mean of -4.58 and the credible interval of (-5.00, -4.18). For the estimation of the true ATE of -5, the GP works better than the BART resulting in the underestimation. These results show that reflecting the bounded feature in the outcome is important in making a correct inference.

Example 7. Estimating ATE for data with multiple imputation for missing values

For generating a simulated incomplete dataset, we randomly selected 50% of records of the dataset in Example 1 and let the predictor X be missing from the selected records. We used the MICE package to get five imputed datasets which are saved in the example8_midata.csv file. By running the code in Listing 27 or Listing 28, we have the results shown in Listing 29 that contains the estimated ATE and potential outcomes for each of five imputed datasets, and the combined results over all five imputations.

```
outcome="Y",
7
                                       treatment = "A",
                                       time="Time",
9
                                       x.explanatory="X",
10
                                       x.confounding="X",
11
                                       burn.num=500,
12
13
                                       mcmc.num=500,
                                       outcome.type="Continuous",
14
                                       method="GP",
                                       tr.type="Discrete",
16
                                       mi.datafile="example7_
17
      midata.csv")
18
status <- pcatsAPIclientR::wait_for_result(jobid)</pre>
20
if (status=="Done") {
cat(pcatsAPIclientR::printgp(jobid))
```

Listing 27: R code of Example 8.

```
import pcats_api_client as pcats_api
2 import requests
4 r = requests.get("https://github.com/pcats-api/
      pcats_api_examples/raw/main/data/example7.csv")
6 with open("example7.csv", 'wb') as f:
      f.write(r.content)
9 r = requests.get("https://github.com/pcats-api/
      pcats_api_examples/raw/main/data/example7_midata.csv")
with open("example7_midata.csv", 'wb') as f:
     f.write(r.content)
12
jobid=pcats_api.staticgp(datafile="example7.csv",
        outcome="Y",
         treatment = "A"
16
         x_explanatory="X",
17
          x_confounding="X",
18
         burn_num=500,
19
         mcmc_num=500,
20
          outcome_type="Continuous",
21
22
          tr_type="Discrete",
          method="GP",
23
          mi_datafile="example7_midata.csv")
24
26 print("JobID: {}".format(jobid))
status=pcats_api.wait_for_result(jobid)
30 if status=="Done":
print(pcats_api.printgp(jobid))
```

```
print("Error")
```

Listing 28: Python code of Example 7.

```
Average treatment effect:
   Imputation Contrast Estimation
                                        SD
                                                LB
                                                        UB
             1 A=0 - A=1
2 A=0 - A=1
                           -5.097 0.344 -5.742 -4.437
                              -5.098 0.346 -5.743 -4.424
             3 A=0 - A=1
                              -5.098 0.344 -5.764 -4.443
5
             4 A = 0 - A = 1
                              -5.098 0.344 -5.773 -4.452
             5 A=0 - A=1
                              -5.097 0.344 -5.729 -4.407
      Combined A=0 - A=1
                              -5.098 0.344 -5.743 -4.415
8
10 Potential outcomes:
11
   Imputation A Estimation
                               SD
                                       LB
                                              UB
            1 0
                     -0.109 0.152 -0.380 0.216
12
                     -0.099 0.152 -0.387 0.217
13
             2 0
                     -0.158 0.144 -0.427 0.144
             3 0
14
             4 0
                     -0.150 0.148 -0.423 0.156
15
                     -0.092 0.154 -0.381 0.230
            5 0
16
                      4.987 0.201 4.613 5.381
4.999 0.202 4.602 5.388
             1 1
17
18
             2 1
             3 1
                      4.940 0.208 4.531 5.350
19
             4 1
                      4.948 0.206 4.558 5.360
20
             5 1
                      5.006 0.200 4.632 5.401
21
                     -0.122 0.152 -0.411 0.197
4.976 0.205 4.584 5.382
      Combined 0
22
      Combined 1
23
24
25 Plot URL: https://pcats.research.cchmc.org/api/job/c0091916-9b9e
       -476e-9ca6-1d76d6dece22/plot
26
27 Plot Potential URL: https://pcats.research.cchmc.org/api/job/
     c0091916-9b9e-476e-9ca6-1d76d6dece22/plot/Potential
```

Listing 29: Result output of Example 7.