

Table 1: Comparison of TMLE and one-step ATE estimators under weak overlap across mediator types.

|        |          | Univariate Binary   |                     | Univariate Continuous |                     |                        |                        |                        |                        | Bivariate Continuous   |                        |                        |                        |
|--------|----------|---------------------|---------------------|-----------------------|---------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
|        |          | $\psi_1(\hat{Q}^*)$ | $\psi_1^+(\hat{Q})$ | $\psi_1(\hat{Q}^*)$   | $\psi_1^+(\hat{Q})$ | $\psi_{2a}(\hat{Q}^*)$ | $\psi_{2a}^+(\hat{Q})$ | $\psi_{2b}(\hat{Q}^*)$ | $\psi_{2b}^+(\hat{Q})$ | $\psi_{2a}(\hat{Q}^*)$ | $\psi_{2a}^+(\hat{Q})$ | $\psi_{2b}(\hat{Q}^*)$ | $\psi_{2b}^+(\hat{Q})$ |
| n=500  | Bias     | -0.004              | -0.01               | -0.022                | -0.004              | -0.002                 | 0                      | -0.002                 | -0.012                 | -0.012                 | 0.153                  | -0.031                 | -0.065                 |
|        | SD       | 0.078               | 0.418               | 0.135                 | 0.799               | 0.432                  | 2.524                  | 0.405                  | 1.191                  | 0.61                   | 5.096                  | 0.495                  | 1.447                  |
|        | MSE      | 0.006               | 0.174               | 0.019                 | 0.638               | 0.187                  | 6.363                  | 0.164                  | 1.418                  | 0.372                  | 25.965                 | 0.245                  | 2.097                  |
|        | Coverage | 91.2%               | 95.4%               | 96.6%                 | 95.2%               | 98.4%                  | 97.1%                  | 98.3%                  | 97.3%                  | 99.4%                  | 98.2%                  | 98.5%                  | 97.7%                  |
|        | CI width | 0.317               | 0.854               | 1.533                 | 1.531               | 4.764                  | 5.705                  | 2.72                   | 3.447                  | 10.115                 | 12.1                   | 2.854                  | 3.834                  |
| n=1000 | Bias     | 0                   | -0.002              | -0.012                | -0.018              | -0.004                 | 0.041                  | -0.003                 | 0.02                   | -0.015                 | -0.078                 | -0.003                 | -0.001                 |
|        | SD       | 0.056               | 0.207               | 0.101                 | 0.47                | 0.342                  | 1.394                  | 0.338                  | 0.787                  | 0.389                  | 1.841                  | 0.333                  | 0.716                  |
|        | MSE      | 0.003               | 0.043               | 0.01                  | 0.221               | 0.117                  | 1.942                  | 0.114                  | 0.619                  | 0.152                  | 3.391                  | 0.111                  | 0.513                  |
|        | Coverage | 92.1%               | 95.4%               | 96%                   | 94.3%               | 98.5%                  | 96.3%                  | 98%                    | 97.1%                  | 99.4%                  | 97.1%                  | 99%                    | 96.4%                  |
|        | CI width | 0.24                | 0.492               | 0.931                 | 0.93                | 3.071                  | 3.46                   | 1.861                  | 2.178                  | 4.809                  | 5.365                  | 1.852                  | 2.136                  |
| n=2000 | Bias     | 0                   | -0.002              | -0.005                | 0.01                | 0.009                  | 0.01                   | 0.009                  | 0.014                  | 0.003                  | -0.006                 | 0.008                  | 0.022                  |
|        | SD       | 0.039               | 0.114               | 0.068                 | 0.239               | 0.238                  | 0.699                  | 0.243                  | 0.481                  | 0.319                  | 0.98                   | 0.276                  | 0.489                  |
|        | MSE      | 0.001               | 0.013               | 0.005                 | 0.057               | 0.057                  | 0.488                  | 0.059                  | 0.231                  | 0.102                  | 0.959                  | 0.076                  | 0.24                   |
|        | Coverage | 94.1%               | 96.2%               | 97.4%                 | 96%                 | 99.2%                  | 96.9%                  | 98.7%                  | 96%                    | 99.2%                  | 96.9%                  | 98.6%                  | 97.4%                  |
|        | CI width | 0.175               | 0.318               | 0.602                 | 0.602               | 1.96                   | 2.092                  | 1.321                  | 1.454                  | 2.989                  | 3.209                  | 1.351                  | 1.504                  |