Online Supplemental Materials to Dynamic Treatment Regimes

Bibhas Chakraborty[1] and Susan A. Murphy[2]

[1]Department of Biostatistics, Columbia University

[2]Department of Statistics and Institute for Social Research, University of Michigan

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1 Simulation Study of Methods for Constructing Confidence Sets

Here we present a simulation study to provide an empirical evaluation of the confidence intervals discussed in Section 4 of the paper *Dynamic Treatment Regimes*; the results are compiled from Laber *et al.* [1] and Chakraborty *et al.* [2]. Nine generative models [3, 1], each having two stages of treatment and two treatments per stage, are used; they can be generically described as: $O_j \in \{-1, 1\}$, $A_j \in \{-1, 1\}$ for $j = 1, 2$; $P(A_j = 1) = 0.5$ for $j = 1, 2$; $P(O_1 = 1) = 0.5$, $P(O_2 = 1|O_1, A_1) = \text{expit}(\delta_1 O_1 + \delta_2 A_1)$; $Y_1 \equiv 0$; $Y_2 = \gamma_1 + \gamma_2 O_1 + \gamma_3 A_1 + \gamma_4 O_1 A_1 + \gamma_5 A_2 + \gamma_6 O_2 A_2 + \gamma_7 A_1 A_2 + \epsilon$, where $\epsilon \sim \mathcal{N}(0, 1)$ and $\text{expit}(x) = \mathrm{e}^x/(1 + \mathrm{e}^x)$. The degree of non-regularity in these models are measured by the following two quantities: (i) $p = P[\gamma_5 A_2 + \gamma_6 O_2 A_2 + \gamma_7 A_1 A_2 = 0]$, and (ii) $\phi = E(\gamma_5 + \gamma_6 O_2 + \gamma_7 A_1)/\sqrt{\text{Var}(\gamma_5 + \gamma_6 O_2 + \gamma_7 A_1)}$.

Table 1: Parameters indexing the example models.

Example	γ^T	δ^T	Type	Non-regularity Measures	
1	$(0, 0, 0, 0, 0, 0, 0)$	$(0.5, 0.5)$	non-regular	$p = 1$	$\phi = 0/0$
2	$(0, 0, 0, 0, 0.01, 0, 0)$	$(0.5, 0.5)$	near-non-regular	$p = 0$	$\phi = \infty$
3	$(0, 0, -0.5, 0, 0.5, 0, 0.5)$	$(0.5, 0.5)$	non-regular	$p = 1/2$	$\phi = 1.0$
4	$(0, 0, -0.5, 0, 0.5, 0, 0.49)$	$(0.5, 0.5)$	near-non-regular	$p = 0$	$\phi = 1.02$
5	$(0, 0, -0.5, 0, 1.0, 0.5, 0.5)$	$(1.0, 0.0)$	non-regular	$p = 1/4$	$\phi = 1.41$
6	$(0, 0, -0.5, 0, 0.25, 0.5, 0.5)$	$(0.1, 0.1)$	regular	$p = 0$	$\phi = 0.35$
7	$(0, 0, -0.25, 0, 0.75, 0.5, 0.5)$	$(0.1, 0.1)$	regular	$p = 0$	$\phi = 1.035$
8	$(0, 0, 0, 0, 0.25, 0, 0.25)$	$(0, 0)$	non-regular	$p = 1/2$	$\phi = 1.00$
9	$(0, 0, 0, 0, 0.25, 0, 0.24)$	$(0, 0)$	near-non-regular	$p = 0$	$\phi = 1.03$

Table 1 provides the parameter settings; they are described as "non-regular," "near-non-regular," and "regular." Ex 1 is a setting where there is no treatment effect for any participant at either stage. Ex 2 is similar to Ex 1 with a very weak stage 2 treatment effect for every participant, but it is hard to detect it given the noise level in the data. Ex 3 is a setting where there is no stage 2 treatment effect for half the participants in the population, but a reasonably large effect for the other half. In Ex 4, there is a very weak stage 2 treatment effect for half the participants in the population, but a reasonably large effect for the other half (the parameters are close to those in Ex 3). Ex 5 is a setting where there is no stage 2 treatment effect for one-fourth of the participants, but others have a reasonably large effect. Ex 6 is a completely regular setting where

there is a reasonably large stage 2 treatment effect for every participant in the population. Ex 7 is an example of a strongly regular setting. Ex 8 is an example of a non-regular setting where the non-regularity is strongly dependent on the stage 1 treatment. In Ex 8, for histories with $A_1 = 1$, there is a moderate effect of A_2 at the second stage, but for histories with $A_1 = -1$, there is no effect of A_2 at the second stage, i.e. both treatments at the second stage are equally optimal. In Ex 9, for histories with $A_1 = 1$, there is a moderate effect of A_2, and for histories with $A_1 = -1$, there is a small effect of A_2; this "near-non-regular" example behaves similar to Ex 8.

The Q-learning analysis models used in the simulation study are given by $Q_2(H_2, A_2; \beta_2, \psi_2) = H_{20}^T\beta_2 + H_{21}^T\psi_2 A_2$, and $Q_1(H_1, A_1; \beta_1) = H_{10}^T\beta_1 + H_{11}^T\psi_1 A_1$, where $H_{20} = (1, O_1, A_1, O_1A_1)^T$, $H_{21} = (1, O_2, A_1)^T$, $H_{10} = (1, O_1)^T$, and $H_{11} = (1, O_1)^T$. Thus the models for the Q-functions are correctly specified. For the purpose of inference, the focus lies on ψ_{10}, the main effect parameter associated with the stage 1 treatment A_1; it can be explicitly expressed in terms of γ's and δ's; see Chakraborty *et al.* [3] for details. Below we will present simulation results to compare the performances of five competing methods of constructing CIs for ψ_{10}. The comparisons are conducted using $N = 1000$ simulated data sets, $B = 1000$ bootstrap replications, and the sample size $n = 300$. We will be reporting the results for *centered percentile* bootstrap (CPB) [4] method defined below. Let $\hat{\theta}$ be an estimator of θ and $\hat{\theta}^{(b)}$ be its bootstrap version. Then the $100(1-\alpha)\%$ CPB confidence interval is given by $\left(2\hat{\theta} - \hat{\theta}^{(b)}_{(1-\frac{\alpha}{2})}, 2\hat{\theta} - \hat{\theta}^{(b)}_{(\frac{\alpha}{2})}\right)$, where $\hat{\theta}^{(b)}_{\gamma}$ is the 100γ-th percentile of the bootstrap distribution. The competing methods are: (i) CPB interval with resample size n (n-CPB); (ii) adaptive confidence interval (ACI) with pretest critical value $\lambda_n = \log\log n$; (iii) m-out-of-n CPB interval with fixed $\eta = 0.05$ (which corresponds to the smallest acceptable resample size of 230 approximately when $n = 300$) ($\hat{m}_{0.05}$-CPB); (iv) m-out-of-n CPB interval with data-driven η chosen by double bootstrap ($\hat{m}_{\hat{\eta}}$-CPB). Both versions of the m-out-of-n bootstrap use a pretest level $\nu = 0.001$, but the performance of the approach has been shown to be robust to this choice; see Chakraborty *et al.* [2] for a detailed sensitivity analysis.

Table 2: Monte Carlo estimates of the coverage probabilities (and the mean widths, within parenthesis) of confidence intervals for ψ_{10} at the 95% nominal level. Estimates significantly below 0.95 at the 0.05 level are marked with $*$. Estimates significantly above 0.95 (conservative) are in bold font. Examples are designated NR = non-regular, NNR = near-non-regular, R = regular.

n=300	Ex. 1 NR	Ex. 2 NNR	Ex. 3 NR	Ex. 4 NNR	Ex. 5 NR	Ex. 6 R	Ex. 7 R	Ex. 8 NR	Ex. 9 NNR
n-CPB	0.936	0.932*	0.928*	0.921*	0.933*	0.931*	0.944	0.925*	0.922*
	(0.269)	(0.269)	(0.300)	(0.300)	(0.320)	(0.309)	(0.314)	(0.299)	(0.299)
ACI	**0.994**	**0.994**	**0.975**	**0.976**	0.962	0.957	0.950	**0.977**	**0.976**
	(0.354)	(0.354)	(0.342)	(0.342)	(0.341)	(0.327)	(0.327)	(0.342)	(0.342)
$\hat{m}_{0.05}$-CPB	0.960	0.963	0.944	0.945	0.936	0.941	0.946	0.951	0.952
	(0.306)	(0.306)	(0.320)	(0.320)	(0.331)	(0.325)	(0.323)	(0.321)	(0.321)
$\hat{m}_{\hat{\eta}}$-CPB	0.964	0.964	0.953	0.950	0.939	0.947	0.944	0.955	0.960
	(0.331)	(0.331)	(0.321)	(0.323)	(0.330)	(0.336)	(0.322)	(0.328)	(0.328)

2 Results

Results are shown in Table 2. n-CPB shows the problem of under-coverage in most of the examples. The ACI is conservative in some of the highly non-regular settings but delivers coverage rates closer to nominal as the settings become more and more regular (as p decreases). Both versions of the m-out-of-n bootstrap provide accurate coverage rates. While the success of the data-driven η version can be expected to be maintained in other generative models, the same may not hold with the fixed-η version for data sets coming from other generative models or at other levels of noise (with larger fixed values of η, the method tends to become conservative). CIs constructed via the usual n-out-of-n bootstrap method (n-CPB) have the least mean width; however these are often associated with under-coverage. The widths of the CIs from ACI and the two versions of the m-out-of-n bootstrap are comparable. In terms of computational cost, n-CPB and $\hat{m}_{0.05}$-CPB are computationally comparable, while ACI and $\hat{m}_{\hat{\eta}}$-CPB are computationally more expensive (each takes about 180 times more computing time than CPB-HM).

Based on the above findings, it may be reasonable to call the m-out-of-n bootstrap method a winner. Both versions of this method perform very well in the set of example generative models we considered. Furthermore, this method is conceptually simple and easy to implement, and hence

may be more attractive to practitioners. The closest competitor is ACI, which is theoretically the strongest (by virtue of its consistency under local alternatives), but is conceptually complicated, and often conservative in finite samples.

References

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