Supplemental Appendix to:

Reproducible Aggregation of Sample-Split Statistics*

David M. Ritzwoller
Stanford University

Joseph P. Romano
Stanford University

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APPENDIX A. DATA AND SIMULATIONS

A.1 Casey et al. (2021b)

We obtain the data associated with Casey et al. (2021a,b) from the replication package posted on OpenICPSR.[28] The units of observation are the aspirant political candidates in Sierra Leone's 2018 parliamentary elections. The data that we consider consist of an outcome and 48 covariates. The outcome is the vote share for each aspirant candidate in a poll of party officials. The covariates collect various measurements relating to the candidate's personal, political, and financial characteristics. All data cleaning steps match Casey et al. (2021b).

We consider the exercise summarized in Appendix Table A.4 of Casey et al. (2021b). These authors repeatedly compute 10-fold cross-validated estimates of the risk associated with a regularized regression of the outcome on the collection of covariates, at each value of a grid of penalization parameters. They include both Ridge and Lasso type penalties. For each replication, they compute the covariates that are selected in the regression associated with the penalty parameter having the minimum risk estimate. They display the covariates that are selected in more than 200 of the 400 replications. These covariates are included as controls in various downstream analyses. In our replication of this exercise, to ease exposition, we only include a Lasso type penalty.

A.2 Chakravorty et al. (2024a)

We obtain the data and replication package associated with Chakravorty et al. (2024a,b) directly from the authors.[29] The units of observation are trainees in a job training program implemented in the Indian states of Bihar and Jharkhand. There are 2,488 total trainees, who were divided into batches of approximately 30 trainees. Batches of trainees were randomly assigned to treatment with a program involving the provision of information concerning potential placement jobs. All data cleaning steps match those taken in Chakravorty et al. (2024a) .

We replicate the analysis reported in Column 4 of Table 1 of Chakravorty et al. (2024a). This estimate restricts attention to the 890 trainees that completed the training and were subsequently placed into a job. The outcome variable is an indicator for whether the trainee is still in the job five months after training completion. The covariates collect measurements of 77 attributes related to the demographics, human capital, and expectations of the trainees. These covariates are listed in Table 3.1 of Chakravorty et al. (2024a).

Following Chakravorty et al. (2024a), we estimate the effect of the treatment using the implementation of Double Machine Learning available through the "DoubleML" R package (Bach et al., 2024). We use 5-fold cross-fitting. Nuisance parameters (i.e., outcome regressions and propensity scores) are

[28] The replication package associated with Casey et al. (2021b) is posted at the URL `https://www.openicpsr.org/openicpsr/project/124501/version/V1/view`.

[29] We thank Bhaskar Chakravorty for sharing this material.

estimated with Random Forests using the default tuning parameters associated with the "Ranger" R package (Wright and Ziegler, 2017). Standard errors are clustered at the batch level.

A.3 Haushofer et al. (2022)

Haushofer et al. (2022) consider data originally studied in Egger et al. (2022a,b). At the time of the preparation of this paper, no replication materials for Haushofer et al. (2022) were publicly available. We replicate a simplified version of the exercise considered in Haushofer et al. (2022), using data obtained from the replication package associated with Egger et al. (2022b).[30] The units of observation are households in three sub-counties of Siaya County, western Kenya. Households were randomly allocated large cash transfers. See Egger et al. (2022b) and Haushofer et al. (2022) for further details on the design of this experiment.

Using the replication data from Egger et al. (2022b,a), we begin with a sample of 5,423 treatment eligible households. We then restrict attention to 4,758 households who were surveyed in both the first and second round of the experiment. We drop any households that are missing measurements of post-treatment assets, consumption, income, or food security, leaving a sample of 4,755 households. These data are merged with pre-treatment measurements of the demographics, assets, food security, and labor market participation for each household, leaving a sample of 4,754 households.

We obtain a cleaned dataset that records 24 measurements associated with each household. The dataset identifies the village that contains each household, whether each household was assigned to treatment, and post-treatment measurements of indices of assets, consumption, income, and food security. The covariates are measurements of the household size, the number of meals eaten the day before the survey, the number of high-protein meals eaten the day before the survey, the time between the administration of the program and the measurement of post-treatment outcomes,[31] and indicators for whether the household contains a widow, contains a female, has children, has children under 3, has children under 6, contains an elderly resident, has livestock, has land, has more than a quarter acre of land, has a radio and tv, has a self-employed resident, and has an employed resident.

We implement a simplified version of the exercise studied in Haushofer et al. (2022). Consider a subset s. Let the complement of s in $[n]$ be denoted by $\tilde{\mathsf{s}}$. Let Y_i denote a measurement of an index quantifying post-treatment consumption, X_i denote a vector of measurements of pre-treatment covariates, and W_i denote assignment to treatment. Let H_i denote the number of occupants of household i. Let D_i collect these observations. Let $Y_i(1)$ and $Y_i(0)$ denote the potential outcomes

[30] The replication package for Egger et al. (2022b) is available at https://www.econometricsociety.org/publications/econometrica/2022/11/01/General-Equilibrium-Effects-of-Cash-Transfers-Experimental-Evidence-From-Kenya.

[31] We use the measurement of the time between the administration of the program and the measurement of post-treatment outcomes available as "exptoend" in the dataset "GE_Survey_and_Transfer_Dates.dta" in the replication package for Egger et al. (2022b). This variable appears to differ from the analogous quantity used in Haushofer et al. (2022), whose density is displayed in their Figure A.2.

induced by the treatment W_i. For each household i in s, let

$$\mathsf{te}(D_i, \hat{\eta}(D_{\tilde{\mathsf{s}}})) \quad \text{and} \quad \mathsf{uto}(D_i, \hat{\eta}(D_{\tilde{\mathsf{s}}})) \tag{A.1}$$

denote sample-split estimates of the treatment effect $Y_i(1) - Y_i(0)$ and *per-capita* untreated outcome $Y_i(0)/H_i$, respectively. In this case, the nuisance parameters $\hat{\eta}(D_{\tilde{\mathsf{s}}})$ consist of nonparametric estimates of outcome regressions, i.e., the conditional expectations (2.7), computed using the data for units i in $\tilde{\mathsf{s}}$.

Following Haushofer et al. (2022), we compute these estimates with Random Forests using the "GRF" R package (Athey et al., 2019).[32] As best as we can tell, there are two differences between our implementation and the results presented in Haushofer et al. (2022). First, we make no attempt to include sample weights that reflect the sampling probabilities. Second, we include the time between treatment and the measurement of post-treatment outcomes as a covariate, rather than implement some form of de-meaning and re-weighing of estimates across time.

Let $\mathsf{Impacted}(\mathsf{s})$ collect the 50% of units in s associated with the largest values of $\mathsf{te}(D_i, \hat{\eta}(D_{\tilde{\mathsf{s}}}))$. Similarly, let $\mathsf{Deprived}(\mathsf{s})$ collect the 50% of units i in s associated with the smallest values of $\mathsf{uto}(D_i, \hat{\eta}(D_{\tilde{\mathsf{s}}}))$. Let $\mathsf{Impacted}_w(\mathsf{s})$ collect the subset of $\mathsf{Impacted}(\mathsf{s})$ with $W_i = w$. Define $\mathsf{Deprived}_w(\mathsf{s})$ analogously. Consider the sample-split statistic

$$\begin{aligned} T(\mathsf{s}, D) = &\left(\frac{1}{|\mathsf{Impacted}_1(\mathsf{s})|} \sum_{i \in \mathsf{Impacted}_1(\mathsf{s})} Y_i - \frac{1}{|\mathsf{Impacted}_0(\mathsf{s})|} \sum_{i \in \mathsf{Impacted}_0(\mathsf{s})} Y_i \right) \\ &- \left(\frac{1}{|\mathsf{Deprived}_1(\mathsf{s})|} \sum_{i \in \mathsf{Deprived}_1(\mathsf{s})} Y_i - \frac{1}{|\mathsf{Deprived}_0(\mathsf{s})|} \sum_{i \in \mathsf{Deprived}_0(\mathsf{s})} Y_i \right) . \end{aligned} \tag{A.2}$$

That is, the sample-split statistic (A.2) is an estimator of the difference in the average treatment effect of the most impacted and most deprived units in s. The statistic (A.2) can be aggregated with cross-splitting, through

$$a(\mathsf{r}, D) = \frac{1}{k} \sum_{i=1}^{k} T(\mathsf{s}_i, D) \ , \tag{A.3}$$

where $\mathsf{r} = (\mathsf{s}_i)_{i=1}^k$ is a k-fold partition of $[n]$. Following Haushofer et al. (2022), in Section 2, we use 5-fold cross-fitting.

Haushofer et al. (2022) say that they construct a standard error for (A.3) with the bootstrap. There are a variety of ways that one might do this. In our implementation, we keep the values of the treatment effect and untreated outcome estimates (A.1) fixed for each household, and compute a

[32] Following Haushofer et al. (2022), we use the default tuning parameters, but set "sample.fraction" equal to 0.1 and "min.node.size" equal to 10.

bootstrap standard error for the statistic (A.3), re-computing the groups $\mathsf{Impacted}(\mathsf{s})$ and $\mathsf{Deprived}(\mathsf{s})$ in each bootstrap replicate.

A.4 Beaman et al. (2023b)

We obtain the data associated with Beaman et al. (2023a,b) from the associated replication package posted on the Econometric Society's webpage.[33] The units of observations are low-income farmers in Mali. The cleaned data consist of observations of 5210 farmers across 198 villages. All data cleaning steps match Beaman et al. (2023b).

Beaman et al. (2023b) consider a two-stage experiment. In the first stage, a microcredit organization randomly offered group-liability loans to women in 88 of the 198 villages. In the second stage, households were randomly offered cash grants. We replicate the analysis reported in Column (4) of Appendix Table VI of Beaman et al. (2023b). In this setting, attention is restricted to the 2,142 households who received a loan. They are interested in testing whether the effects of cash-grants on farm profits are heterogeneous. For this problem, the data D_i consist of a measurement Y_i of the post-transfer profit for farm i, the variable W_i denotes assignment to the cash transfer, and the vector X_i collects a vector of pre-treatment measurements of the physical and financial attributes of each farm. Let $Y_i(1)$ and $Y_i(0)$ denote the potential outcomes induced by the treatment W_i.

Beaman et al. (2023b) implement a sample-split test for treatment effect heterogeneity proposed by Chernozhukov et al. (2023). Let s denote a random half-sample of $[n]$, i.e., a random subset of $[n]$ of size $n/2$. As before $\tilde{\mathsf{s}}$ denotes the complement of s in $[n]$. For each farm i in s, let

$$\mathsf{te}(D_i, \hat{\eta}(D_{\tilde{\mathsf{s}}})) \tag{A.4}$$

denote sample-split estimates of the treatment effect $Y_i(1) - Y_i(0)$. The nuisance parameters $\hat{\eta}(D_{\tilde{\mathsf{s}}})$ consist of nonparametric estimates of outcome regressions, i.e., the conditional expectations (2.7), computed using the data for units i in $\tilde{\mathsf{s}}$. We compute these estimates with Random Forests using the "GRF" R package (Athey et al., 2019). Tuning parameters are chosen with cross-validation in the same manner implemented in Beaman et al. (2023b).

To test for treatment effect heterogeneity, we estimate the coefficients of the linear regression

$$Y_i = \alpha + \tau_1 \cdot W_i + \tau_2 \cdot \mathsf{te}(D_i, \hat{\eta}(D_{\tilde{\mathsf{s}}})) + \tau_3 \cdot W_i \cdot \mathsf{te}(D_i, \hat{\eta}(D_{\tilde{\mathsf{s}}})) + \varepsilon_i \,. \tag{A.5}$$

The idea is that, if the treatment effect estimates are heterogeneous, then the "true" value of the interaction coefficient τ_3 should be positive. Let $\hat{\tau}_3(\mathsf{s}, D)$ denote the estimate of τ_3 computed with linear regression in the sample s. Let $\mathsf{se}(\mathsf{s}, D)$ denote the associated standard error, clustered at the

[33] The replication package for Beaman et al. (2023b) is available at https://www.econometricsociety.org/publications/econometrica/2023/09/01/Selection-into-Credit-Markets-Evidence-from-Agriculture-in-Mali

village level. Chernozhukov et al. (2023) advocate for computing the median estimate and standard error over 250 half-splits s. Beaman et al. (2023b) use 1000 half-splits.

A.5 Simulations

In this section, we give further details concerning the simulations whose results are reported in Section 4. For both the applications to Casey et al. (2021b) and Chakravorty et al. (2024a), we sample 100,000 replications of the cross-split statistic of over a range of values of k. In the application to Chakravorty et al. (2024a), we have increased the number of trees used to compute the random forest nuisance parameter estimates, from 100 to 3000, in order to ensure that the residual randomness induced by cross-splitting is greater than the residual randomness induced by the nuisance parameter estimate. We use these replicates to estimate the variance $v_{1,k}(D)$ for each value of k, in addition to the oracle stopping time

$$g^\star = 2v_{1,k}(D)\left(\frac{z_{1-\beta/2}}{\xi}\right)^2, \tag{A.6}$$

at each value of k and ξ

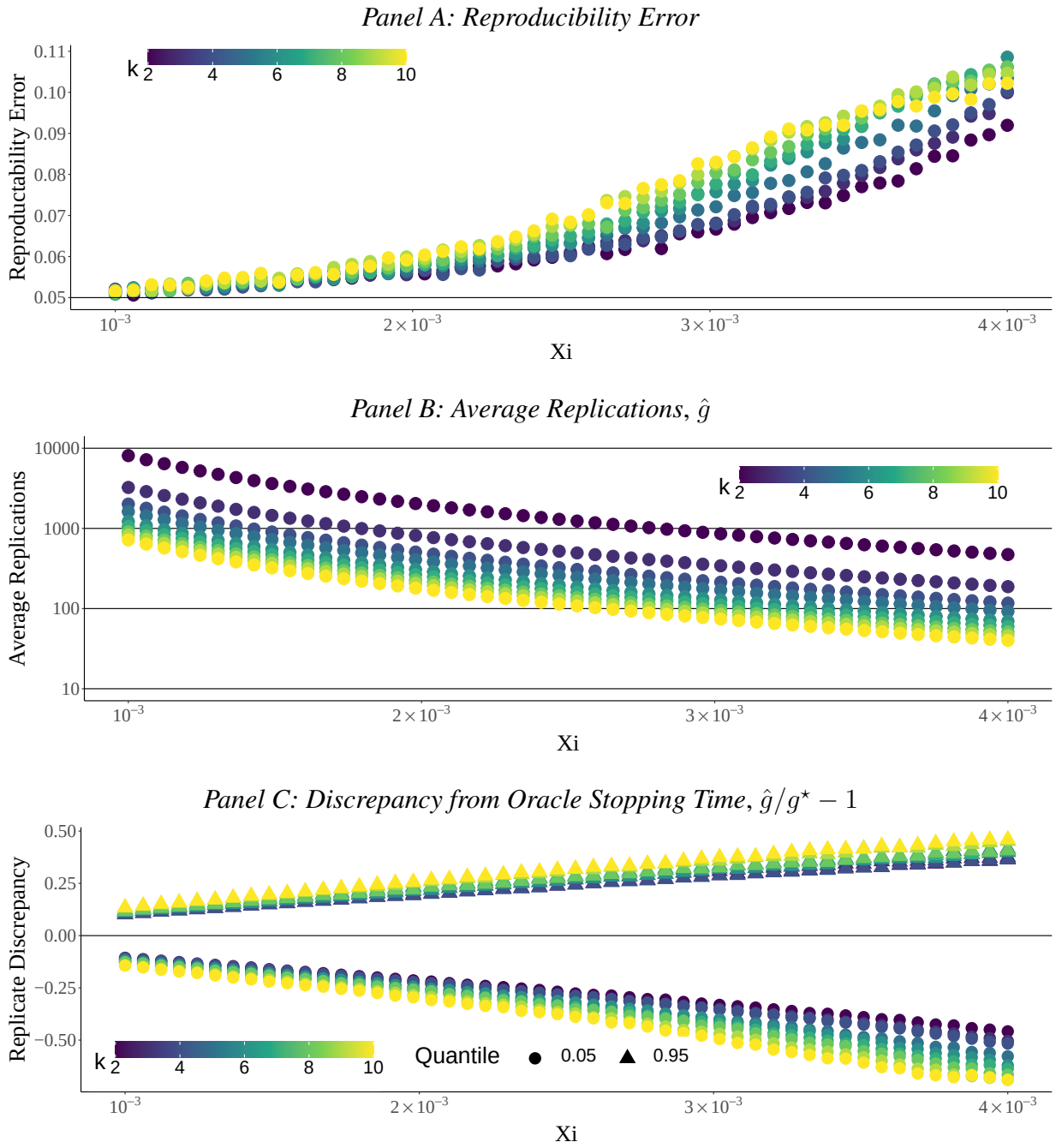
We implement Algorithm 1 100,000 times for each value of k and ξ, for each application, by sampling with replacement from the replicates of 100,000 draws. We use these estimates to estimate the reproducibility error

$$P\left\{\left|a(\mathsf{R}_{\hat{g},k}, D) - a(\mathsf{R}'_{\hat{g}',k}, D)\right| \geq \xi \mid D\right\} \tag{A.7}$$

as well as the distribution of $\hat{g}$ for each k and ξ. These estimates are used to construct Figure 5.

Figure A.1 displays measurements analogous to those displayed in Figure 5 for the application to Chakravorty et al. (2024a). The accuracy of the reproducibility error, relative to the application to Casey et al. (2021b), is somewhat worse. This is likely a consequence of the fact that the quality of a normal approximation to the conditional distribution of the p-value (3.11) is worse than the quality of the normal approximation to the conditional distribution of the mean-squared error estimate. As before, the reproducibility error tends to be most accurate at values of k and ξ where the average number of cross-splits $\hat{g}$ is greater than 500.

FIGURE A.1. Performance in Application to Chakravorty et al. (2024a)



Notes: Figure A.1 displays measurements of the performance of Algorithm 1 on the data from Chakravorty et al. (2024a). Panel A displays measurements of the reproducibility error, $P\{|a(\mathsf{R}_{\hat{g},k}, D) - a(\mathsf{R}'_{\hat{g}',k}, D)| \geq \xi \mid D\}$, as ξ and k vary. A solid horizontal line is displayed at the nominal error rate $\beta = 0.05$. Panel B displays measurements of the average number of replications $\hat{g}$ s ξ and k vary. The y-axis is displayed with a log scale, base 10. Solid horizontal lines are placed at each exponential factor of 10. Panel C displays measurements of the 0.05th and 0.95th quantiles of the discrepancy $\hat{g}/g^\star - 1$ as k and ξ vary. Further details on the construction of this figure are given in Appendix A.5.

APPENDIX B. AUXILIARY RESULTS AND DISCUSSION

B.1 Validity of Testing Procedures Based on Multiple Sample-Splitting

In this appendix, we discuss the application of Algorithm 1 to testing procedures based on averaging over multiple splits of the same sample. We show that methods based on both p-values and e-values constructed with sample splitting continue to control the Type I error rate if they are aggregated sequentially with Algorithm 1. Both results follow from the "Exchangeable Markov Inequality" of Ramdas and Manole (2023). As before, let $D = (D_i)_{i=1}^n$ be independent and identically distributed according to a probability distribution P. Interest is in testing the null hypothesis $H_0 : P \in \mathbf{P}$ for some collection of probability distributions $\mathbf{P}$.

B.1.1 Methods Based on p-Values. Suppose that we have access to a valid p-value $\hat{p}(\mathsf{s}, D)$. That is, the statistic $\hat{p}(\mathsf{s}, D)$ satisfies

$$P\left\{\hat{p}(\mathsf{s}, D) \leq u \mid D_{\tilde{\mathsf{s}}}\right\} \leq u$$

for all u in $(0, 1)$ and P in $\mathbf{P}$. For example, a test-statistic could be chosen using the data in $D_{\tilde{\mathsf{s}}}$ and a p-value can be constructed based on this test statistic using the data in D_{s}. For any collection $\mathsf{R}_{g,k}$ in $\mathcal{R}_{n,k,b}$, let

$$a_\delta(\mathsf{R}_{g,k}, D) = \frac{1}{g}\frac{1}{k}\sum_{i=1}^{g}\sum_{j=1}^{k}\mathbb{I}\left\{\hat{p}(\mathsf{s}_{i,j}, D) \leq \delta\right\} \tag{B.1}$$

denote the proportion of p-values that are less than or equal than δ. Rüger (1978), Meinshausen et al. (2009), and DiCiccio et al. (2020) observe that if $\mathsf{R}_{g,k}$ is constructed independently of the data D, then

$$P\left\{a_\delta(\mathsf{R}_{g,k}, D) \geq c\right\} \leq \frac{\mathbb{E}\left[a_\delta(\mathsf{R}_{g,k}, D)\right]}{c} \leq \frac{\delta}{c}$$

by Markov's inequality, for all P in $\mathbf{P}$. Thus, if δ and c are chosen such that $\delta/c = \alpha$, then the test that rejects the null hypothesis H_0 if $a_\delta(\mathsf{R}_{g,k}, D)$ is larger than c has level α.

The following theorem establishes that this test continues to be valid if the collection of sample-splits $\mathsf{R}_{g,k}$ is constructed sequentially with Algorithm 1.

Theorem B.1. *If the statistic $a_\delta(\mathsf{R}_{\hat{g},k}, D)$ defined in (B.1) is constructed sequentially with Algorithm 1, then*

$$P\left\{a_\delta(\mathsf{R}_{\hat{g},k}, D) \geq c\right\} \leq \frac{\delta}{c} \tag{B.2}$$

for all P in $\mathbf{P}$.

Proof. We apply the following inequality, due to Ramdas and Manole (2023).

Theorem B.2 (Theorem 1.1, Ramdas and Manole (2023))**.** *If $X_1, X_2, \ldots$ form an exchangeable sequence of integrable random variables, then*

$$P\left\{\exists t \geq 1 : \frac{1}{t}\sum_{i=1}^{t} |X_i| \geq 1/a\right\} \leq a\mathbb{E}\left[|X_i|\right] \tag{B.3}$$

for any $a > 0$.

Consequently, we have that

$$\begin{aligned} P\left\{a_\delta(\mathsf{R}_{\hat{g},k}, D) \geq c\right\} &\leq P\left\{\exists g \geq 1 : a_\delta(\mathsf{R}_{g,k}, D) \geq c\right\} \\ &\leq \frac{\mathbb{E}\left[\mathbb{I}\left\{\hat{p}(\mathsf{s}_{i,j}, D) \leq \delta\right\}\right]}{c} \leq \frac{\delta}{c} \end{aligned} \tag{B.4}$$

by Theorem B.2, as required. ■

B.1.2 Methods Based on e-Values. Next, we consider settings where we have access to a valid e-value $\hat{e}(\mathsf{s}, D)$ (see Ramdas et al. (2023) for a recent review). That is, the nonnegative statistic $\hat{e}(\mathsf{s}, D)$ satisfies

$$\mathbb{E}_P\left[\hat{e}(\mathsf{s}, D)\right] \leq 1$$

for all P in $\mathbf{P}$. For example, this setting applies to the "Universal Inference" procedure of Wasserman et al. (2020). Here, an estimator $\hat{P}(\tilde{\mathsf{s}})$ of P is formed using the data $D_{\tilde{\mathsf{s}}}$ and is used in the split-likelihood ratio test statistic

$$\hat{e}(\mathsf{s}, D) = \inf_{P \in \mathbf{P}} \prod_{i \in \mathsf{s}} \frac{\mathrm{d}\hat{P}(\tilde{\mathsf{s}})}{\mathrm{d}P}(D_i) \,. \tag{B.5}$$

Wasserman et al. (2020) prove that (B.5) is an e-value. For any collection $\mathsf{R}_{g,k}$ in $\mathcal{R}_{n,k,b}$, let

$$a(\mathsf{R}_{g,k}, D) = \frac{1}{g}\frac{1}{k}\sum_{i=1}^{g}\sum_{j=1}^{k} \hat{e}(\mathsf{s}_{i,j}, D) \tag{B.6}$$

denote an aggregate e-value. See Dunn et al. (2023) and Tse and Davison (2022) for further discussion of aggregate e-values. Observe that

$$P\left\{a(\mathsf{R}_{g,k}, D) \geq 1/\alpha\right\} \leq \alpha\mathbb{E}\left[\hat{e}(\mathsf{s}, D)\right] \leq \alpha \,, \tag{B.7}$$

by Markov's inequality, for all P in $\mathbf{P}$. Thus, the test that rejects the null hypothesis H_0 if $a(\mathsf{R}_{g,k}, D)$ is larger than $1/\alpha$ has level α.

We again establish that this test continues to be valid if the collection of sample splits $\mathsf{R}_{g,k}$ is constructed sequentially with Algorithm 1.

Theorem B.3. *If the aggregate e-value $a_\delta(\mathsf{R}_{\hat{g},k}, D)$ defined in (B.6) is constructed sequentially with Algorithm 1, then*

$$P\left\{a(\mathsf{R}_{\hat{g},k}, D) \geq \frac{1}{\alpha}\right\} \leq \alpha \tag{B.8}$$

for all P in $\mathbf{P}$.

Proof. The claim is established with an argument very similar to the proof of Theorem B.1. Namely, the Markov inequality used to establish (B.7) can then be replaced by Theorem B.2, as before. ■

B.2 Determining Suitable Levels of Precision for Cross-Validated Risk Estimation

In this section, we give the details supporting our application of Algorithm 1 to cross-validated risk estimation, using data from Casey et al. (2021b). Recall from Section 3.2.2, that we apply the procedure, independently, to each component of the vector

$$(b_{\lambda_1}(\mathsf{r}, D), \ldots, b_{\lambda_{p-1}}(\mathsf{r}, D)) \,, \quad \text{where} \quad b_{\lambda_i}(\mathsf{r}, D) = (a_{\lambda_i}(\mathsf{r}, D) - a_{\lambda_p}(\mathsf{r}, D)) \,. \tag{B.9}$$

Let ξ_i denote the error tolerance used for the ith component of the vector (B.9). We use a simple, data-driven procedure for choosing these tolerances.

In particular, we draw a small number of cross-splits, i.e., $g = 20$ and compute the aggregated difference

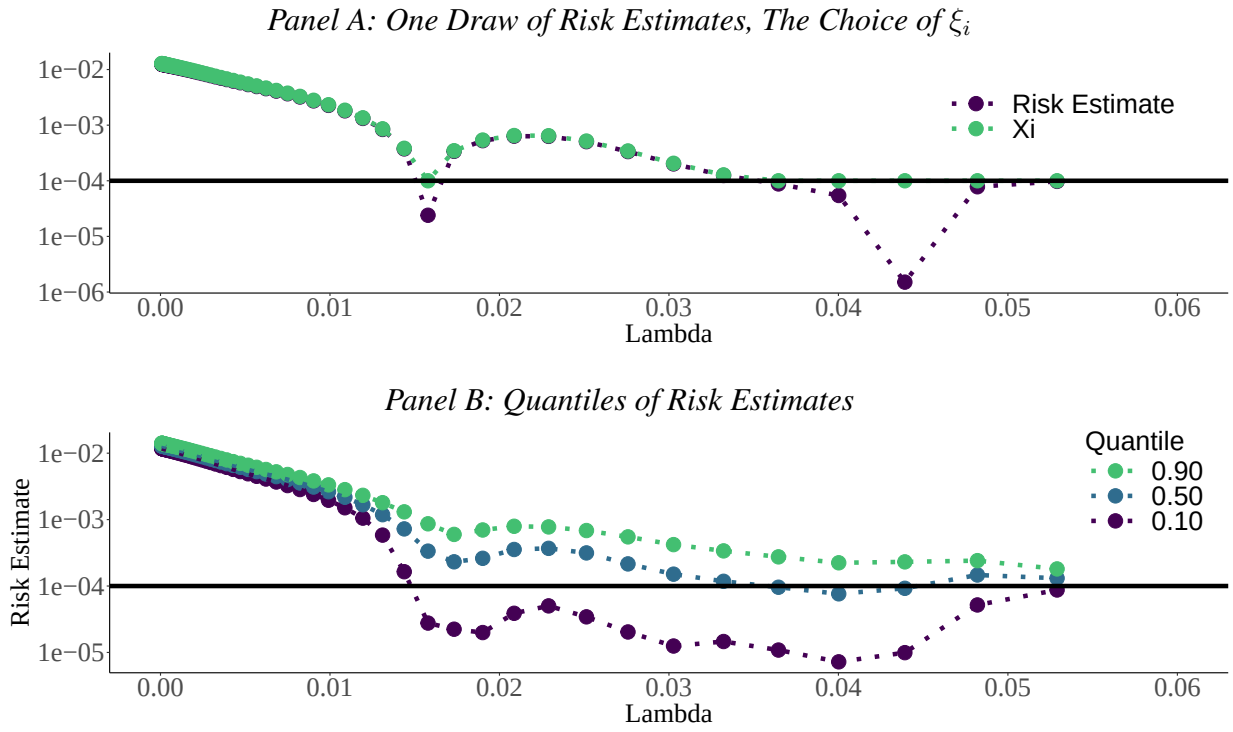
$$b_{\lambda_i}(\mathsf{R}_{g,k}, D) = \frac{1}{g}\sum_{i=1}^{g} b_{\lambda_i}(\mathsf{r}_i, D) \tag{B.10}$$

for each i in $1, \ldots, p-1$. Panel A of Figure B.2 displays the absolute value of these estimates in purple, where the y-axis has been transformed to a logarithmic scale. The absolute value of the differences (B.10) are on the order 10^{-4} at the close-to-optimal values of λ, i.e., values of λ above about 0.01. The differences for smaller values of λ are much larger, and, as indicated by Figure 1, have larger conditional variances. These qualitative features are not particularly sensitive to residual randomness. Panel B of Figure B.2 displays the quantiles of the difference (B.10) across draws of $g = 20$ cross-splits.

These observations suggest the following approach for choosing the tolerances ξ_i. We would like to set $\xi_i = 10^{-4}$ for the large, close-to-optimal values of the regularization parameter, but would be willing to tolerate a larger error tolerance at smaller, sub-optimal values. This is practically important, as achieving the same level of precision for the small values of λ requires aggregation over many more cross-splits (as the conditional variances are much larger). We operationalize this approach in the following way. First, using the sample of $g = 20$ cross-splits that we used to estimate (B.10), we compute the p-values

$$q_{\lambda_i}(\mathsf{R}_{g,k}, D) = 1 - \Phi\left(\frac{b_{\lambda_i}(\mathsf{R}_{g,k}, D)}{\sqrt{\hat{v}_{\lambda_i}(\mathsf{R}_{g,k}, D)}}\right) \tag{B.11}$$

FIGURE B.2. Determining Error Tolerances for Cross-Validated Risk Estimation



Notes: Figure B.2 displays auxiliary measurements relating to the the performance of Algorithm 1 in the application to cross-validated Lasso, implemented in data from Casey et al. (2021b). Panel A displays the absolute value of the differences (B.10) computed on a random sample of $g = 20$ cross-splits, in purple, and the realized values of the error tolerances (B.13), in green. Panel B displays the quantiles of the absolute value of the differences (B.10), over replications of random samples of $g = 20$ cross-splits. In both cases, the y-axes is displayed in a logarithmic scale.

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for each i in $1, \ldots, p-1$, where $\hat{v}_{\lambda_i}(\mathsf{R}_{g,k}, D)$ denotes the sample-variance of the statistics $b_{\lambda_i}(\mathsf{r}_i, D)$ across the sample-splits. Let $\overline{\lambda}$ denote the largest value of the regularization parameter such that $q_{\overline{\lambda}}(\mathsf{R}_{g,k}, D) < 0.2$ and let the constant "scale" solve the equality

$$10^{-4} = \frac{b_{\overline{\lambda}}(\mathsf{R}_{g,k}, D)}{\mathsf{scale}} \,. \tag{B.12}$$

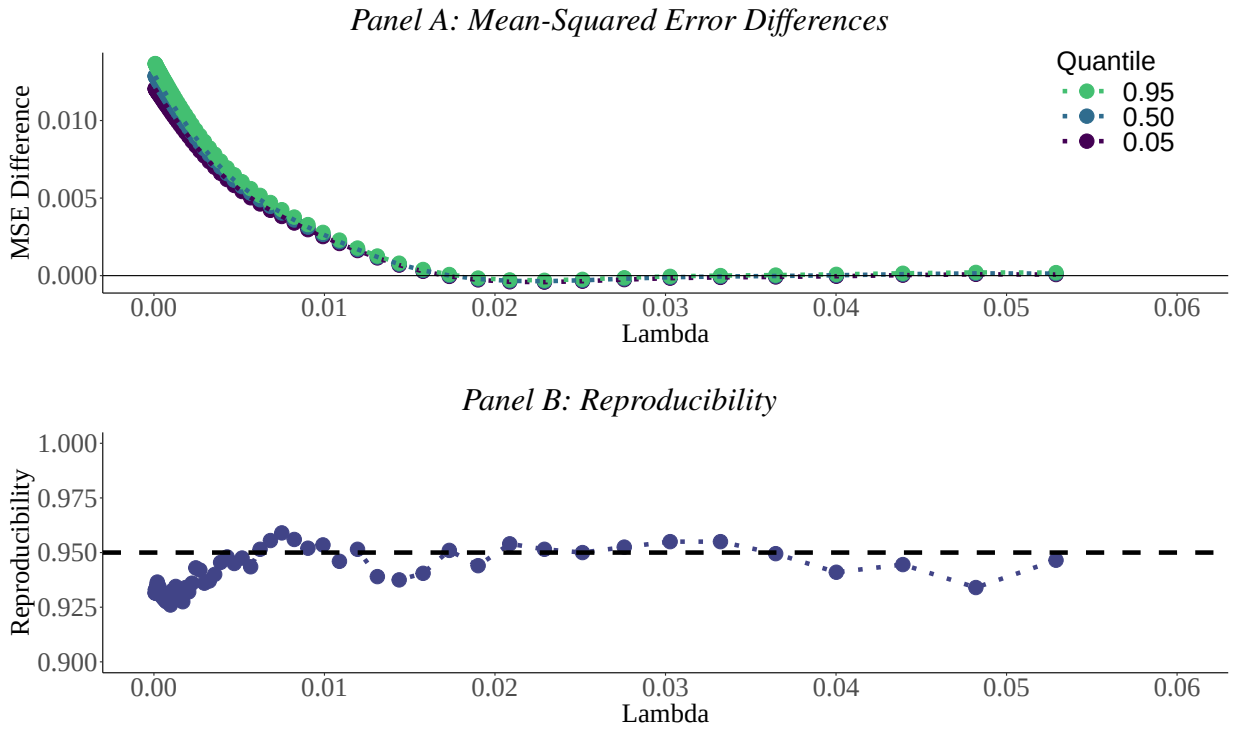
We set the error tolerances to

$$\xi_i = \max\{10^{-4}, b_{\lambda_i}(\mathsf{R}_{g,k}, D) \times \mathsf{scale}\} \,. \tag{B.13}$$

In other words, we set $\xi_i = 10^{-4}$ for all i with $q_{\lambda_i}(\mathsf{R}_{g,k}, D) \geq 0.2$ and increase the error tolerance in proportion to $b_{\lambda_i}(\mathsf{R}_{g,k}, D)$ for all other values of i. The realized values of ξ_i are displayed in Panel A of Figure B.2. These error tolerances are used throughout the main text.

Panel A displays quantiles of the reproducibly aggregated statistic (3.12) across replications of the procedure, without truncation of the y-axis. Panel B of Figure B.2 displays estimates of the marginal reproducibility probability at each value of the regularization parameter, computed

FIGURE B.3. Auxiliary Figures for Application to Cross-Validation



Notes: Figure B.2 displays auxiliary measurements relating to the the performance of Algorithm 1 in the application to cross-validated Lasso, implemented in data from Casey et al. (2021b). Panel A is analogous to Panel A of Figure 3, but the y-axis is not truncated. Panel B displays estimates of the marginal reproducibility probability for each value of the regularization parameter, where the nominal reproducibility error is set to $\beta = 0.05$.

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using $2,000$ replications of the procedure. Over the full range of the regularization parameter, the reproducibility error is very close to the nominal value $\beta = 0.05$.

B.3 Sample Stability

This appendix collects discussion and analysis concerning the (r, q)-sample stability $\sigma^{(r,q)}$ defined in Definition 4.1. First, in Appendix B.3.1, we specialized our consideration to the case that the estimator $\hat{\eta}$ is a regularized empirical risk minimizer. Some closely related arguments are used in proof of Proposition 4 of Austern and Zhou (2020). Second, in Appendix B.3.2 we compare we compare the stable-stability decay condition Assumption 4.3 to the conditions considered by Chen et al. (2022). The proof of the Theorem stated in Appendix B.3.1 is given in Appendix B.3.3

B.3.1 Specialization to Regularized Empirical Risk Minimizers. Assume that the parameter η is an element of some closed convex space $H \subseteq \mathbb{R}^p$. Consider the estimator

$$\Psi\left(D_{\mathsf{s}}, \eta\right) = \frac{1}{b} \sum_{i \in \mathsf{s}} \psi\left(D_i, \eta\right) \tag{B.14}$$

$$\hat{\eta} = \underset{\eta \in H}{\arg\min} \left\{ \frac{1}{n-b} \sum_{i \in \tilde{\mathsf{s}}} \ell\left(D_i, \eta\right) + \lambda_{1,n} \|\eta\|_1 + \lambda_{2,n} \|\eta\|_2 \right\}, \tag{B.15}$$

where $\psi\left(\cdot,\cdot\right)$ are $\ell\left(\cdot,\cdot\right)$ functions and $\lambda_{1,n}, \lambda_{2,n} \geq 0$ are penalty parameters.

Let $\nabla \ell\left(d,\eta\right)$ and $\nabla^2 \ell\left(d,\eta\right)$ denote the gradient and Hessian of the function $\eta \mapsto \ell\left(d,\eta\right)$. Let $\nabla_j \ell\left(\cdot,\cdot\right)$ denote the jth component of $\nabla \ell\left(\cdot,\cdot\right)$. Similarly, we write

$$\overline{\nabla}_{\tilde{\mathsf{s}}} \ell\left(D,\eta\right) = \frac{1}{n-b} \sum_{i \in \tilde{\mathsf{s}}} \nabla \ell\left(D_i,\eta\right) \quad \text{and}$$

$$\overline{\nabla}^2_{\tilde{\mathsf{s}}} \ell\left(D,\eta\right) = \frac{1}{n-b} \sum_{i \in \tilde{\mathsf{s}}} \nabla^2 \ell\left(D_i,\eta\right)$$

for the empirical averages of the gradients and the Hessian evaluated on the data in the set $\tilde{\mathsf{s}}$.

We impose the following set of restrictions. The first two restrictions concern the curvature of the loss function.

Assumption B.1. *The minimum eigenvalue of $\overline{\nabla}^2_{\tilde{\mathsf{s}}} \ell\left(D,\eta\right)$ is bounded below by ρ almost surely.*

Assumption B.2. *The loss function $\ell\left(\cdot,\cdot\right)$ is strictly convex and twice continuously differentiable in its second argument.*

Remark B.1. Under Assumption B.1, if $\rho > 0$, then the dimension p of the parameter vector η is less than the number of observations n. To the best of our knowledge, analysis of the stability of ℓ_1 regularized empirical risk minimization in the regime with p larger than n is an open problem. Further analysis of the sample stability in the high-dimensional regime is an interesting direction for further research. ■

The second two restrictions are statistical. The first concerns the expected curvature of the moment function $\psi\left(\cdot,\cdot\right)$. The second is a sub-exponential tail bound on the gradient $\nabla_j \ell\left(\cdot,\cdot\right)$.

Assumption B.3. *The function $\psi\left(\cdot,\cdot\right)$ satisfies the inequality*

$$\mathbb{E}\left[\left(\psi(D_i,\eta) - \psi(D_i,\eta')\right)^r\right] \lesssim \mathbb{E}\left[\|\hat{\eta} - \hat{\eta}'\|_2^r\right] \tag{B.16}$$

for each pair $\eta, \eta' \in H$.

Assumption B.4. *The ψ_1-Orlicz norm bound*

$$\|\nabla_j \ell_j(D_i',\eta) - \nabla_j \ell(D_i,\eta)\| \lesssim \kappa^2 \tag{B.17}$$

holds for each pair $\eta \in H$.

Remark B.2. Assumption B.3 is satisfied in many problems of interest. For example, Chen et al. (2022) show that similar conditions hold when $\psi(\cdot,\cdot)$ is given by various moment functions

used for semiparametric causal inference. Assumption B.4 is equivalent to the assumption that $\nabla_j \ell_j(D_i', \eta) - \nabla \ell_j(D_i, \eta)$ is sub-exponential with parameter κ^2. ■

The following theorem gives a bound on the (r, q)-sample stability.

Theorem B.4. *If Assumptions B.1 to B.4, if $\rho + \lambda_{2,n} > 0$, then*

$$\sigma^{(r,q)} \lesssim C_r p \left(\frac{\sqrt{q}}{n-b} \frac{\kappa}{\rho + \lambda_{2,n}} \right)^r + C_r \left(\lambda_{1,n} \frac{p}{\rho + \lambda_{2,n}} \right)^r ,$$

uniformly over all even integers r and positive integers $q \leq n - b$, where C_r is some positive constant that depends only on r.

Remark B.3. A necessary and sufficient condition for $\hat{\eta}$ to be consistent for the population risk minimizer associated with (B.15) is that $\lambda_{1,n} = o\left((n-b)^{-1}\right)$. See e.g., Knight and Fu (2000). Thus, so long as the penalty $\lambda_{1,n}$ is chosen in this regime, the sample stability $\sigma^{(r,q)}$ will be

$$O\left(\left(\frac{\sqrt{q}\kappa}{n-b} \right)^r \right)$$

up to terms that depend on the dimension of η, as required. ■

B.3.2 Comparison to Chen et al. (2022). In the main text, we restrict attention to sample stable estimators. In a recent article, Chen et al. (2022) show that, under some regularity conditions, if a condition related to, but partially stronger than, sample stability is satisfied, then sample-splitting is unnecessary for the consistency and asymptotic normality of DML estimators. In this section, we comment on the difference between the notion of sample stability used in this article and the related condition used in Chen et al. (2022).

First, for ease of reference, we recall our definition of sample stability. We restrict attention to the case that $q = 1$ and $r = 2$, as this is what is relevant to make the comparison. Fix a set $\mathsf{s} \subseteq \mathcal{S}_{n,b}$ and let i be an arbitrary element of s. Let D' denote an independent and identical copy of the data D. For each i in $[n]$, let $\tilde{D}^{(i)}$ be constructed by replacing D_i with D_i' in D. Let I be a randomly selected element of $\tilde{\mathsf{s}}$. In this paper, we refer to the quantity

$$\sigma^{(2,1)} = \mathbb{E}\left[\left(\psi(D_i, \hat{\eta}\left(D_{\tilde{\mathsf{s}}}\right)) - \psi(D_i, \hat{\eta}(\tilde{D}^{(I)}_{\tilde{\mathsf{s}}})) \right)^2 \right] \tag{B.18}$$

as the $(2,1)$-sample stability. In particular, in the main text, we restrict attention to settings where the bound

$$\sigma^{(2,1)} \lesssim \left(\frac{1}{n-b} \right)^2 \tag{B.19}$$

holds.

Chen et al. (2022) consider settings where the nuisance parameter estimator $\hat{\eta}$ is not constructed with sample-splitting. Likewise, they consider moments of the form

$$\tilde{\sigma}^{(2,1)} = \mathbb{E}\left[\left(\psi(D_i, \hat{\eta}\,(D)) - \psi(D_i, \hat{\eta}(\tilde{D}^{(i)}))\right)^2\right] , \tag{B.20}$$

where i is an arbitrary element of $[n]$. Observe that, in contrast to (B.18), the moment (B.20) is evaluated using the same observation D_i used to perturb the nuisance parameter estimate—and that the nuisance parameter estimate is evaluated using the complete data. Roughly speaking, Chen et al. (2022) show that, under some regularity conditions, DML estimators are consistent and asymptotically normal if the bound

$$\tilde{\sigma}^{(2,1)} \lesssim n^{-1} \tag{B.21}$$

holds for a suitable choice of the function $\psi(\cdot, \cdot)$. Moreover, they show that, under certain conditions on the choice of tuning parameters, nuisance parameter estimators constructed with a bagged 1-nearest-neighbor estimator satisfies this bound.

Although the right-hand-side of the bound (B.21) is larger than the bound (B.19), control of the moment (B.20) can be more difficult to achieve than control of the moment (B.18). To see the substantive differences between the conditions (B.19) and (B.20), we consider an artificial, but illustrative, example adapted from an example given in the introduction to Chernozhukov et al. (2018). Suppose that the observation D_i consists of the real-valued quantities Y_i, W_i, and X_i. Furthermore, suppose that the nuisance parameter $\eta(x)$ denotes the conditional expectation $\mathbb{E}[W_i \mid X_i = x]$ and that

$$\psi(D_i, \eta) = Y_i(W_i - \mathbb{E}[W_i \mid X_i]) = Y_i(W_i - \eta(x)) . \tag{B.22}$$

Suppose that the nuisance parameter estimator takes the form

$$\hat{\eta}(D_{\tilde{\mathsf{s}}})(x) = \sum_{j \in \tilde{\mathsf{s}}} w_j(x)\hat{\eta}_j(x) \tag{B.23}$$

where $\tilde{\mathsf{s}}$ is an arbitrary subset of $[n]$, $\hat{\eta}_j(x)$ is an estimator of the nuisance parameter $\eta(x)$ based on the observation D_j, and the weight $w_j(x)$ again depends on the observation D_j and the set $\tilde{\mathsf{s}}$. We refer the reader to discussion in Section 1 of Chernozhukov et al. (2018) and Section 2 of Chen et al. (2022) for further context on why understanding quantities of the form (B.22) is essential for establishing the consistency of DML estimators.[34]

To study the sample stability (B.18) in this example, i.e., in the sense considered in this article, we are interested in the difference

$$\psi(D_i, \hat{\eta}\,(D_{\tilde{\mathsf{s}}})) - \psi(D_i, \hat{\eta}(\tilde{D}^{(I)}_{\tilde{\mathsf{s}}})) = Y_i(w_I(X_i)\hat{\eta}_I(X_i) - w'_I(X_i)\hat{\eta}'_I(X_i)) \tag{B.24}$$

[34] In particular, establishing the Stochastic Equicontinuity of a given Neyman Orthogonal moment amounts to bounding scaled averages of quantities of the form (B.22).

where $w'_I(X_i)$ and $\hat{\eta}'_I(X_i))$ denote the updated weight and estimator associated with the perturbed data $\tilde{D}^{(I)}_{\tilde{\mathsf{s}}}$. On the other hand, in order to consider the stability (B.20), i.e., in the sense of Chen et al. (2022), we are interested in the difference

$$\psi(D_i, \hat{\eta}\,(D)) - \psi(D_i, \hat{\eta}(\tilde{D}^{(i)})) = Y_i(w_i(X_i)\hat{\eta}_i(X_i) - w'_i(X_i)\hat{\eta}'_i(X_i)) \tag{B.25}$$

where, as before, $w'_i(X_i)$ and $\hat{\eta}'_i(X_i)$ denote the updated weight and estimator associated with the perturbed data $\tilde{D}^{(i)}$.

The quantities (B.24) and (B.25) will behave differently if the nuisance parameter estimator exhibits overfitting. In particular, to take a highly stylized example, suppose that the weights satisfy

$$w_i(X_j) = \begin{cases} |\tilde{\mathsf{s}}|^{-1/3}, & i = j, \\ |\tilde{\mathsf{s}}|^{-1}, & \text{otherwise.} \end{cases} \tag{B.26}$$

That is, the nuisance parameter estimator (B.23) meaningfully up-weights the estimate obtained from the evaluation point X_j, if X_j is part of the training data $\tilde{\mathsf{s}}$, and is otherwise equally balanced. Overfitting to the training data, in a perhaps less stylized form, is a well-known property of some machine learning estimators.

It is easy to see that, in this case, if all other quantities are bounded, we should expect that

$$\begin{aligned} \sigma^{(2,1)} &= \mathbb{E}\left[\left(\psi(D_i, \hat{\eta}\,(D_{\tilde{\mathsf{s}}})) - \psi(D_i, \hat{\eta}(\tilde{D}^{(I)}_{\tilde{\mathsf{s}}}))\right)^2\right] \\ &= \mathbb{E}\left[\left(Y_i(w_I(X_i)\hat{\eta}_I(X_i) - w'_I(X_i)\hat{\eta}'_I(X_i))\right)^2\right] \lesssim \left(\frac{1}{|\tilde{\mathsf{s}}|}\right)^2 \end{aligned} \tag{B.27}$$

whereas

$$\begin{aligned} \tilde{\sigma}^{(2,1)} &= \mathbb{E}\left[\left(\psi(D_i, \hat{\eta}\,(D)) - \psi(D_i, \hat{\eta}(\tilde{D}^{(i)}))\right)^2\right] \\ &= \mathbb{E}\left[\left(Y_i(w_i(X_i)\hat{\eta}_i(X_i) - w'_i(X_i)\hat{\eta}'_i(X_i))\right)^2\right] \lesssim \left(\frac{1}{|\tilde{\mathsf{s}}|}\right)^{2/3}. \end{aligned} \tag{B.28}$$

In particular, we can see that all that is needed for us to expect the moment (B.27) to be approximately of order $O((n-b)^{-2})$, is that the *randomly selected* weights $w_I(X_i)$ *tend* to be close to, or smaller than, $(n-b)^{-1}$. The moment (B.28), by contrast, is highly sensitive to the weight $w_i(X_i)$ placed on the evaluation point X_i.

The main point of this example is that establishing that a nuisance parameter estimator is stable, in the sense of Chen et al. (2022), requires showing that it does not overfit its training data, i.e., that evaluations of points *in-sample* are not overly-determined by a few observations. By contrast, all that is needed to establish that a nuisance parameter estimator is sample stable, in the sense used in this article, is that evaluations of points *out-of-sample* are not overly concentrated on a small

number of training samples. In general, we should expect that out-of-sample balance is more likely to occur in practice than in-sample balance.

B.3.3 Proof of Theorem B.4. By Assumptions B.1 and B.2, the objective function for the estimator (B.15) is strongly convex. Thus, there is a unique solution to (B.15) for any data D. Let $\hat{\eta}$ and $\hat{\eta}'$ denote the solutions to (B.15) for the data D and $\tilde{D}^{(\mathsf{q})}$ respectively. Let $\partial f(x)$ denote the subgradient set of the function $x \mapsto f(x)$. The Karush-Kuhn-Tucker condition for the program (B.15) is given by

$$\overline{\nabla}_{\tilde{\mathsf{s}}} \ell(D, \eta) + \lambda_{2,n} \hat{\eta} + \lambda_{1,n} \hat{z} = 0, \tag{B.29}$$

where $\hat{z} \in \partial \|\hat{\eta}\|_1$ is the subgradient associated with the Lasso penalty. Observe that, in this case, $\hat{z} \in \text{sign}(\hat{\eta})$, where we set $\text{sign}(0) = [-1, 1]$. Let $\hat{z}$ and $\hat{z}'$ denote the subgradients obtained from D and $\tilde{D}^{(\mathsf{q})}$, respectively. As $\ell(d, \cdot)$ is twice continuously differentiable under Assumption B.2 (i), we have that

$$\begin{aligned}
&\overline{\nabla}_{\tilde{\mathsf{s}}} \ell(D, \hat{\eta}') + \lambda_{2,n} \hat{\eta}' + \lambda_{1,n} \hat{z} \\
&= \overline{\nabla}_{\tilde{\mathsf{s}}} \ell(D, \hat{\eta}) + \lambda_{2,n} \hat{\eta} + \lambda_{1,n} \hat{z} + \left(\overline{\nabla}^{(2)}_{\tilde{\mathsf{s}}} \ell(D, \tilde{\eta}) + \lambda_{2,n} I_d \right) (\hat{\eta} - \hat{\eta}') \\
&= \left(\overline{\nabla}^{(2)}_{\tilde{\mathsf{s}}} \ell(D, \tilde{\eta}) + \lambda_{2,n} I_d \right) (\hat{\eta} - \hat{\eta}')
\end{aligned} \tag{B.30}$$

for some vector $\tilde{\eta}$, by a Taylor expansion and the optimality condition (B.29). On the other hand, we have that

$$\begin{aligned}
\overline{\nabla}_{\tilde{\mathsf{s}}} \ell(D, \hat{\eta}') + \lambda_{2,n} \hat{\eta}' + \lambda_{1,n} \hat{z} &= \overline{\nabla}_{\tilde{\mathsf{s}}} \ell(\tilde{D}^{(\mathsf{q})}, \hat{\eta}') + \lambda_{2,n} \hat{\eta}' + \lambda_{1,n} \hat{z}' \\
&\quad + \frac{1}{n-b} \left(\sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \right) + \lambda_{1,n} (\hat{z} - \hat{z}') \\
&= \frac{1}{n-b} \left(\sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \right) + \lambda_{1,n} (\hat{z} - \hat{z}')
\end{aligned} \tag{B.31}$$

again by the optimality condition (B.29). Thus, we have that

$$\begin{aligned}
&\left(\overline{\nabla}^{(2)}_{\tilde{\mathsf{s}}} \ell(D, \tilde{\eta}) + \lambda_{2,n} I_p \right) (\hat{\eta} - \hat{\eta}') \\
&= \frac{1}{n-b} \left(\sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \right) + \lambda_{1,n} (\hat{z} - \hat{z}')
\end{aligned} \tag{B.32}$$

by (B.30) and (B.31). Observe that the the matrix $\overline{\nabla}^{(2)}_{\tilde{\mathsf{s}}} \ell(D, \tilde{\eta}) + \lambda_{2,n} I_p$ is invertible by Assumption B.1. Thus, we find that

$$\hat{\eta} - \hat{\eta}' = \frac{1}{n-b} \left(\overline{\nabla}^{(2)} \ell(D, \tilde{\eta}) + \lambda_2 I_p \right)^{-1} \left(\sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \right)$$

$$+ \lambda_{1,n} \left(\overline{\nabla}^{(2)} \ell \left(D, \tilde{\eta} \right) + \lambda_2 I_d \right)^{-1} (\hat{z} - \hat{z}')$$

and that consequently

$$\begin{aligned} \|\hat{\eta} - \hat{\eta}'\|_2 &\lesssim \frac{1}{n-b} \frac{\| \sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \|_2}{\rho + \lambda_{2,n}} + \lambda_{1,n} \frac{\|\hat{z} - \hat{z}'\|_2}{\rho + \lambda_{2,n}} \\ &\lesssim \frac{1}{n-b} \frac{\| \sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \|_2}{\rho + \lambda_{2,n}} + \lambda_{1,n} \frac{p}{\rho + \lambda_{2,n}} \end{aligned} \tag{B.33}$$

by Assumption B.1.

Now, observe that

$$\begin{aligned} \sigma^{(r,q)} &= \mathbb{E}\left[\left(\psi(D_i, \hat{\eta}) - \psi(D_i, \hat{\eta}') \right)^r \right] \\ &\lesssim \mathbb{E}\left[\|\hat{\eta} - \hat{\eta}'\|_2^r \right] \\ &\lesssim \mathbb{E}\left[\left(\frac{1}{n-b} \frac{\| \sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \|_2}{\rho + \lambda_{2,n}} + \lambda_{1,n} \frac{p}{\rho + \lambda_{2,n}} \right)^r \right] \qquad \text{(B.34)} \\ &\lesssim 2^r \left(\frac{1}{n-b} \frac{1}{\rho + \lambda_{2,n}} \right)^r \mathbb{E}\left[\| \sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \|_2^r \right] \\ &\quad + 2^r \left(\lambda_{1,n} \frac{p}{\rho + \lambda_{2,n}} \right)^r , \qquad \text{(B.35)} \end{aligned}$$

where the first inequality follows from Assumption B.3, the second inequality follows from (B.33), and the third inequality follows from the Binomial Theorem and Cauchy-Schwarz. By Assumption B.4, we have that

$$\| \sum_{i \in \mathsf{q}} \nabla_j \ell_j(D_i', \hat{\eta}') - \nabla \ell_j(D_i, \hat{\eta}') \|_{\psi_1} \lesssim q \| \nabla_j \ell_j(D_i', \hat{\eta}') - \nabla \ell_j(D_i, \hat{\eta}') \|_{\psi_1} \lesssim q\kappa \, . \tag{B.36}$$

Consequently, we have that

$$\begin{aligned} &\mathbb{E}\left[\| \sum_{i \in \mathsf{q}} \nabla \ell(D_i', \hat{\eta}') - \nabla \ell(D_i, \hat{\eta}') \|_2^r \right] \\ &\lesssim \sum_{j \in [p]} \mathbb{E}\left[\left| \sum_{i \in \mathsf{q}} \nabla_j \ell_j(D_i', \hat{\eta}') - \nabla \ell_j(D_i, \hat{\eta}') \right|^{r/2} \right] \qquad \text{(Jensen)} \\ &\lesssim p((r/2)!)^{r/2} (\kappa q)^{r/2} \qquad \text{(B.37)} \end{aligned}$$

where, for the final inequality, we have used the fact that $\|X\|_{r/2} \lesssim ((r/2)!) \|X\|_{\psi_1}$ (see e.g., Section 2.2 of Van Der Vaart and Wellner (1996)). Putting the pieces together, we find that

$$\sigma^{(r,q)} \lesssim 2^r ((r/2)!)^{r/2} p \left(\frac{q^{1/2}}{n-b} \frac{\kappa^{1/2}}{\rho + \lambda_{2,n}} \right)^r + 2^r \left(\lambda_{1,n} \frac{p}{\rho + \lambda_{2,n}} \right)^r , \tag{B.38}$$

as required. ■

APPENDIX C. PROOFS FOR RESULTS STATED IN SECTION 3

C.1 Proof of Theorem 3.1

For each collection $\mathsf{r} = (\mathsf{s}_j)_{j=1}^k$ in $\mathcal{R}_{n,k,b}$, we write

$$\overline{a}(\mathsf{r}, D) = \frac{1}{k}\sum_{j=1}^{k} T(\mathsf{s}_j, D) - \mathbb{E}\left[T(\mathsf{s}_j, D) \mid D\right].$$

Define the oracle stopping time

$$g^\star = \arg\min_{g \geq 2} \left\{ v_{g,k}(D) \leq \frac{1}{2}\left(\frac{\xi}{z_{1-\beta/2}}\right)^2 \right\}.$$

Observe that $v_{g,k}(D) = (1/g) \cdot v_{1,k}(D)$ as the collections of cross-splits are drawn independently and identically. Moreover, we have that

$$\frac{\hat{v}(\mathsf{R}_{g,k}, D)}{v_{g,k}(D)} = \frac{g\hat{v}(\mathsf{R}_{g,k}, D)}{v_{1,k}(D)} \xrightarrow{\text{a.s}} 1 \tag{C.1}$$

as $g \to \infty$, by the strong law of large numbers. Now, observe that

$$\frac{\hat{g} \cdot \hat{v}(\mathsf{R}_{\hat{g},k}, D)}{v_{1,k}(D)} \leq \frac{\hat{g}}{2v_{1,k}(D)}\left(\frac{\xi}{z_{1-\beta/2}}\right)^2 \leq \frac{\hat{g} \cdot \hat{v}(\mathsf{R}_{\hat{g}-1,k}, D)}{v_{1,k}(D)}, \tag{C.2}$$

by definition. Consequently, as $\hat{g} \to \infty$ and

$$g^\star\left(2v_{1,k}(D)\left(\frac{z_{1-\beta/2}}{\xi}\right)^2\right) \to 1$$

as $\xi \to 0$, we have that

$$\hat{g}/g^\star \xrightarrow{\text{a.s}} 1 \tag{C.3}$$

as $\xi \to 0$ by (C.1) and (C.2).

Define the objects

$$U\left(\mathsf{R}_{g,k}, D\right) = \frac{1}{g^\star}\left(\sum_{i=1}^{g} \overline{a}\left(\mathsf{r}_i, D\right) - \sum_{i=1}^{g^\star} \overline{a}\left(\mathsf{r}_i, D\right)\right) \quad \text{and} \tag{C.4}$$

$$Q\left(\mathsf{R}_{g,k}, D\right) = \left(1 - \frac{g}{g^\star}\right)\left(a(\mathsf{R}_{g,k}, D) - \mathbb{E}\left[T(\mathsf{s}_j, D) \mid D\right]\right) \tag{C.5}$$

Observe that we can decompose

$$\left(a(\mathsf{R}_{\hat{g},k}, D) - a(\mathsf{R}'_{\hat{g}',k}, D)\right) / \sqrt{2v_{g^\star,k}(D)}$$

$$= \sqrt{\frac{g^\star}{2v_{1,k}(D)}}\left(a(\mathsf{R}_{g^\star,k}, D) - a(\mathsf{R}'_{g^\star,k}, D)\right)$$

$$+ \sqrt{\frac{g^\star}{2v_{1,k}(D)}}\left(U(\mathsf{R}_{\hat{g},k}, D) - U(\mathsf{R}'_{\hat{g}',k}, D)\right) + \sqrt{\frac{g^\star}{2v_{1,k}(D)}}\left(Q(\mathsf{R}_{\hat{g},k}, D) - Q(\mathsf{R}'_{\hat{g}',k}, D)\right). \quad \text{(C.6)}$$

First, we have that

$$\sqrt{\frac{g^\star}{2v_{1,k}(D)}}\left(Q(\mathsf{R}_{\hat{g},k}, D) - Q(\mathsf{R}'_{\hat{g}',k}, D)\right) = o_p(1)$$

almost surely as $\xi \to 0$ by (C.3). To handle the terms involving (C.4), fix $\varepsilon > 0$ and observe that

$$\begin{aligned}
&P\left\{\left|\sum_{i=1}^{\hat{g}} a(\mathsf{r}_i, D) - \sum_{i=1}^{g^\star} a(\mathsf{r}_i, D)\right| > \varepsilon\sqrt{g^\star} \mid D\right\} \\
&\leq P\left\{\left|\sum_{i=1}^{\hat{g}} a(\mathsf{r}_i, D) - \sum_{i=1}^{g^\star} a(\mathsf{r}_i, D)\right| > \varepsilon\sqrt{g^\star}, \hat{g} \in \left[g^\star\left(1-\varepsilon^3\right), g^\star\left(1+\varepsilon^3\right)\right] \mid D\right\} \\
&+ P\left\{\left|\sum_{i=1}^{\hat{g}} a(\mathsf{r}_i, D) - \sum_{i=1}^{g^\star} a(\mathsf{r}_i, D)\right| > \varepsilon\sqrt{g^\star}, \hat{g}' \notin \left[g^\star\left(1-\varepsilon^3\right), g^\star\left(1+\varepsilon^3\right)\right] \mid D\right\} \\
&\leq P\left\{\max_{g^\star(1-\varepsilon^3)\leq g\leq g^\star}\left|\sum_{i=1}^{g} a(\mathsf{r}_i, D)\right| > \varepsilon\sqrt{g^\star} \mid D\right\} \\
&+ P\left\{\max_{g^\star\leq g\leq(1+\varepsilon^3)g^\star}\left|\sum_{i=1}^{g} a(\mathsf{r}_i, D)\right| > \varepsilon\sqrt{g^\star} \mid D\right\} \\
&+ P\left\{\hat{g} \notin \left[g^\star\left(1-\varepsilon^3\right), g^\star\left(1+\varepsilon^3\right)\right] \mid D\right\}.
\end{aligned} \quad \text{(C.7)}$$

The third term in (C.7) is smaller than ε for all sufficiently small ξ by (C.3). To handle the first two terms, observe that

$$\begin{aligned}
&P\left\{\max_{g^\star\leq g\leq(1+\varepsilon^3)g^\star}\left|\sum_{i=1}^{g} a(\mathsf{r}_i, D)\right| > \varepsilon\sqrt{\hat{g}} \mid D\right\} \\
&\leq \frac{1}{\varepsilon^2}\frac{1}{g^\star}\operatorname{Var}\left(\sum_{i=1}^{\lfloor\varepsilon^3 g^\star\rfloor} a(\mathsf{r}_i, D) \mid D\right) \\
&\leq \varepsilon \operatorname{Var}(a(\mathsf{r}_i, D)),
\end{aligned}$$

almost surely, where the first inequality follows from Kolmogorov's maximal inequality (see e.g., Proposition 2.3.16 of Dembo (2021)) and the second inequality follows from the fact that the cross-splits r_i are independent. An analogous bound holds for the remaining term. Thus, we have

$$\sqrt{\frac{g^\star}{2v_{1,k}(D)}}\left(U(\mathsf{R}_{\hat{g},k}, D) - U(\mathsf{R}'_{\hat{g}',k}, D)\right) = o_p(1)$$

almost surely as $\xi \to 0$. Hence, we have that

$$\begin{aligned}
&P\left\{\left|a(\mathsf{R}_{\hat{g},k}, D) - a(\mathsf{R}'_{\hat{g}',k}, D)\right| > \xi \mid D\right\} \\
&= P\left\{\left|\sqrt{\frac{g^\star}{2v_{1,k}(D)}}\left(\frac{1}{g^\star}\sum_{i=1}^{g^\star} a(\mathsf{r}_{i,k}, D) - a(\mathsf{r}'_{i,k}, D)\right)\right| > z_{1-\beta/2} \mid D\right\} + o\left(1\right) \\
&= 1 - \beta + o\left(1\right)
\end{aligned}$$

as $\xi \to 0$ almost surely, by the central limit theorem. ■

C.2 Proof of Theorem 3.2

Recall that the cross-split r is drawn independently and uniformly from the collection $\mathcal{R}_{n,k,b}$. The result is based on the bound

$$\begin{aligned}
\mathbb{E}\left[f(a(\mathsf{R}_{g,k}, D))\right] &= \mathbb{E}\left[\mathbb{E}\left[f\left(\frac{1}{\hat{g}}\sum_{i=1}^{\hat{g}} a(\mathsf{r}_i, D)\right) \mid \hat{g}\right]\right] \\
&\leq \mathbb{E}\left[\mathbb{E}\left[\frac{1}{\hat{g}}\sum_{i=1}^{\hat{g}} f\left(a(\mathsf{r}_i, D)\right) \mid \hat{g}\right]\right] \qquad \text{(Jensen)} \\
&= \mathbb{E}\left[\frac{1}{\hat{g}}\sum_{i=1}^{\hat{g}} f\left(a(\mathsf{r}_i, D)\right)\right] \\
&= \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right)\right] + \mathbb{E}\left[\frac{1}{\hat{g}}\sum_{i=1}^{\hat{g}}\left(f\left(a(\mathsf{r}_i, D)\right) - \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) \mid D\right]\right)\right]. \qquad \text{(C.8)}
\end{aligned}$$

In particular, it will suffice to show that the second term in (C.8) is weakly negative. To do this, we apply the following optimal stopping theorem.

Theorem C.1 (Theorem 5.7.5, Durrett (2019))**.** *Suppose that X_g is a real-valued supermartingale, that $\mathcal{F}_g$ is the σ-algebra generated by $X_1, \ldots, X_g$, and that there exists some constant B such that*

$$\mathbb{E}\left[|X_{g+1} - X_g| \mid \mathcal{F}_g\right] \leq B \qquad \text{(C.9)}$$

almost surely. If $\hat{g}$ is a stopping time with respect to the filtration $\{\mathcal{F}_g\}_{g=1}^{\infty}$, then $\mathbb{E}\left[X_{\hat{g}}\right] \leq \mathbb{E}\left[X_1\right]$.

Consider the sequence of random variables

$$X_g = \frac{1}{g}\sum_{i=1}^{g}\left(f\left(a(\mathsf{r}_i, D)\right) - \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) \mid D\right]\right) \qquad \text{(C.10)}$$

Observe that

$$\mathbb{E}\left[X_{g+1} \mid \mathcal{F}_g, D\right] = \mathbb{E}\left[\frac{1}{g+1}\sum_{i=1}^{g+1}\left(f\left(a(\mathsf{r}_i, D)\right) - \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) \mid D\right]\right) \mid \mathcal{F}_g, D\right]$$

$$= \frac{1}{g+1}\mathbb{E}\left[f\left(a(\mathsf{r}_i, D)\right) - \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) \mid D\right] \mid \mathcal{F}_g, D\right]$$
$$+ \frac{g}{g+1}\frac{1}{g}\sum_{i=1}^{g}\left(f\left(a(\mathsf{r}_i, D)\right) - \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) \mid D\right]\right)$$
$$= \frac{g}{g+1}X_g\,. \tag{C.11}$$

Consequently, X_g is a supermartingale. To verify the condition (C.9), observe that, as the collection $\mathcal{R}_{n,k,b}$ is finite, there exists some positive, finite function $B(D)$ such that

$$f(a(\mathsf{r}, D)) \leq B(D) \tag{C.12}$$

almost surely. Thus, we find that

$$\mathbb{E}\left[|X_{g+1} - X_g| \mid \mathcal{F}_g, D\right] = \mathbb{E}\left[\left|\frac{1}{g+1}\sum_{i=1}^{g+1} f\left(a(\mathsf{r}_i, D)\right) - \frac{1}{g}\sum_{i=1}^{g} f\left(a(\mathsf{r}_i, D)\right)\right| \mid \mathcal{F}_g, D\right]$$
$$\leq \frac{1}{g+1}\mathbb{E}\left[|f\left(a(\mathsf{r}, D)\right)|\right] + \frac{1}{g(g+1)}\sum_{i=1}^{g}\mathbb{E}\left[|f\left(a(\mathsf{r}_i, D)\right)|\right]$$
$$\leq \frac{2}{g+1}B(D) \tag{C.13}$$

almost surely. Hence, by Theorem C.1, we have

$$\mathbb{E}\left[\frac{1}{\hat{g}}\sum_{i=1}^{\hat{g}}\left(f\left(a(\mathsf{r}_i, D)\right) - \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) \mid D\right]\right) \mid D\right]$$
$$\leq \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) - \mathbb{E}\left[f\left(a(\mathsf{r}, D)\right) \mid D\right] \mid D\right] = 0 \tag{C.14}$$

almost surely, completing the proof. ■

APPENDIX D. GENERAL NON-ASYMPTOTIC RESULTS

In this appendix, we give a general, non-asymptotic analysis of the performance of Algorithm 1. We begin, in Appendix D.1, by studying the concentration and normal approximation of the aggregate statistic $a(\mathsf{R}_{k,g}, D)$. Equipped with these results, in Appendix D.2, we characterize the accuracy of the nominal error rate of Algorithm 1. In Appendix D.3, we show that these general results imply the results stated in Section 4, by restricting attention to sample-stable, cross-split statistics. Proofs are given in Appendices D.4 and D.5.

D.1 Concentration and Normal Approximation

We begin by giving a non-asymptotic characterization of the concentration and normal approximation of the statistic $a(\mathsf{R}_{g,k}, D)$. To state these results, we require a slightly more general definition of sample stability.

Definition D.1 (General Sample Stability)**.** Let D' denote an independent and identical copy of the data D. For each $\mathsf{q} \subseteq [n]$, let $\tilde{D}^{(\mathsf{q})}$ be constructed by replacing D_i with D'_i in D for each i in q. Fix a set $\mathsf{s} \subseteq \mathcal{S}_{n,b}$. Let i be an arbitrary element of s. Let q be a randomly selected subset of $\tilde{\mathsf{s}}$ of cardinality q. We refer to the quantities

$$\sigma^{(r)}_{\mathsf{valid}} = \mathbb{E}\left[\left|\psi(D_I, \hat{\eta}\left(D_{\mathsf{s}}\right)) - \psi(D'_I, \hat{\eta}\left(D_{\tilde{\mathsf{s}}}\right))\right|^r\right] \quad \text{and}$$
$$\sigma^{(r,q)}_{\mathsf{train}} = \mathbb{E}\left[\left|\psi(D_i, \hat{\eta}\left(D_{\mathsf{s}}\right)) - \psi(D_i, \hat{\eta}(\tilde{D}^{(\mathsf{q})}_{\tilde{\mathsf{s}}}))\right|^r\right]$$

as the rth-order validation and (r, q)th-order training sample stabilities, respectively. Similarly, we refer to the quantity

$$\sigma^{(r)}_{\mathsf{max}} = \max\left\{\sigma^{(r)}_{\mathsf{valid}}, \sigma^{(r,1)}_{\mathsf{train}}\right\} \tag{D.1}$$

as the rth-order full sample stability.

In other words, we define separate stabilities associated with resampling data in the subsets s and $\tilde{\mathsf{s}}$. We refer to these subsets as the "validation" and "training" samples, respectively. The training sample stability $\sigma^{(r,q)}_{\mathsf{train}}$ is identical to the sample stability defined in Section 4.

With this in place, we give a large deviations bound for the statistic $a(\mathsf{R}_{g,k}, D)$ about its conditional mean. The primary difficulty is accommodating the dependence in the summands of $a(\mathsf{R}_{g,k}, D)$ across elements of the same cross-split. We tackle this problem through the method of exchangeable pairs (Stein, 1986). In particular, we construct a suitable exchangeable pair with a coupling argument due to Chatterjee (2005) and apply a method for deriving concentration inequalities with exchangeable pairs, also due to Chatterjee (2005, 2007). Some preliminary results that facilitate the application of this approach are given in Appendix D.4. Proofs for results stated in this appendix are then given in Appendix D.5.

Theorem D.1. *Suppose that Assumptions 4.1 and 4.2 hold, that the data D are independently and identically distributed, and that the statistic $a(\mathsf{R}_{1,k}, D)$ has a non-zero variance conditional on D almost surely. If the fourth-order split stability $\zeta^{(4)}$ is finite, then, for each $\varepsilon > 0$, the inequality*

$$P\left\{\left|a(\mathsf{R}_{g,k}, D) - \overline{a}\left(D\right)\right| \leq \sqrt{\frac{2^4(2-\varphi k-\varphi)^2}{\delta}\frac{\Gamma_{k,\varphi,b}\log(\varepsilon^{-1})}{g}} \mid D\right\} \geq 1 - \frac{\varepsilon}{2} \tag{D.2}$$

holds with probability greater than $1-\delta$ as D varies, where

$$\Gamma_{k,\varphi,b} = \left(\frac{1-k\varphi}{1-\varphi}\right)4\sigma^{(2)}_{\mathsf{max}} + \left(\frac{k\varphi-\varphi}{1-\varphi}\right)\sigma^{(2,b-1)}_{\mathsf{train}} \tag{D.3}$$

and $\varphi = b/n$.

Remark D.1. The quantity $\Gamma_{k,\varphi,b}$ interpolates between $\sigma^{(2)}_{\mathsf{max}}$ and $\sigma^{(2,b-1)}_{\mathsf{train}}$ as k varies between its bounds 1 and $1/\varphi$. In the case of independent splitting, i.e., $k = 1$, the rate of concentration

for the statistic $a(\mathsf{R}_{g,k}, D)$ is driven by the full sample stability $\sigma^{(2)}_{\mathsf{max}}$. On the other hand, in the case of cross-splitting, concentration depends only on the training sample stability $\sigma^{(2,b-1)}_{\mathsf{train}}$. In a previous draft of this paper, we give estimates of $\sigma^{(2)}_{\mathsf{valid}}$ and $\sigma^{(2,b-1)}_{\mathsf{train}}$ in applications to treatment effect estimation and cross-validated risk estimation. We show that the training stability is dramatically smaller than the validation stability and decreases rapidly as b decreases.[35] To see this, observe that we should next expect the validation sample-stability $\sigma^{(r)}_{\mathsf{valid}}$ to change with k. That is, residual randomness is smaller for full cross-splitting, i.e., $k = n/b$, than for independent splitting. ■

Next, we derive bounds for the centered conditional moments of $a\left(\mathsf{R}_{g,k}, D\right)$ through an argument closely related to the proof of Theorem D.1. Bounds of this form are known as Burkholder-Davis-Gundy inequalities (Burkholder, 1973).

Theorem D.2. *Suppose that Assumptions 4.1 and 4.2 hold and that the data D are independent and identically distributed. If $r = 2^{c-1}$ for some positive integer c and the $4r$th-order split stability $\zeta^{(4r)}$ is finite, then, for each $\delta >$, the inequality*

$$\mathbb{E}\left[\left(a\left(\mathsf{R}_{g,k}, D\right) - \overline{a}\left(D\right)\right)^{2r} \mid D\right] \leq (2r-1)^r \left(\frac{2^4(2-\varphi k-\varphi)^2}{g}\right)^r \Gamma^{(r)}_{k,\varphi,b}\,, \tag{D.4}$$

holds with probability greater than $1-\delta$ as D varies, where

$$\Gamma^{(r)}_{k,\varphi,b} = \left(\frac{1-k\varphi}{1-\varphi}\right) 2^{2r}\sigma^{(2r,1)}_{\mathsf{max}} + \left(\frac{k\varphi-\varphi}{1-\varphi}\right)\sigma^{(2r,b-1)}_{\mathsf{valid}} \tag{D.5}$$

and $\varphi = b/n$.

Remark D.2. By setting $r = 1$, the inequality (D.4) gives a variance bound. In this case, the right-hand side of the inequality (D.4) is equal to negative one times the inverse of the right-hand side of the inequality (D.2). In this sense, the concentration inequality Theorem D.1 can be thought of as an exponential Efron-Stein inequality adapted to the dependence inherent in our problem (Boucheron et al., 2003). For values of r greater than 1, the unconditional quantity $\Gamma^{(r)}_{k,\varphi,b}$ again interpolates between the $2r$th order full sample stability $\sigma^{(2r,1)}_{\mathsf{max}}$ and the $(2r, b-1)$th order training sample stability $\sigma^{(2r,b-1)}_{\mathsf{valid}}$ as k increases from 1 to $1/\varphi$. ■

Remark D.3. An analogous, unconditional, result will follow from the same argument. In particular, under the same conditions, we have that

$$\mathbb{E}\left[\left(a\left(\mathsf{R}_{g,k}, D\right) - \overline{a}\left(D\right)\right)^{2r}\right] \leq (2r-1)^r \left(\frac{2^4(2-\varphi k-\varphi)^2}{g}\right)^r \Gamma^{(r)}_{k,\varphi,b}\,. \tag{D.6}$$

We opt to state the conditional version of the result thought, as, arguably, the conditional behavior of the statistic is of primary interest. ■

[35] See Figure 3 of the preprint posted at https://arxiv.org/abs/2311.14204v2.

In turn, we bound the distance between the conditional distribution of $a\left(\mathsf{R}_{g,k}, D\right)$ and the standard normal distribution. The result follows by combining the bounds derived in Theorem D.2 with a standard Berry-Esseen inequality (Shevtsova, 2011).

Theorem D.3. *Suppose that Assumptions 4.1 and 4.2 hold, that the data D are independently and identically distributed, and that the statistic $a(\mathsf{R}_{1,k}, D)$ has a non-zero variance conditional on D almost surely. If the eighth-order split stability $\zeta^{(8)}$ is finite, then for all g, the inequality*

$$\sup_{z\in\mathbb{R}}\left|P\left\{\frac{a\left(\mathsf{R}_{g,k}, D\right)-\overline{a}\left(D\right)}{\sqrt{v_{g,k}\left(D\right)}}\leq z \mid D\right\}-\Phi(z)\right| \lesssim \frac{2^6 3^2}{\delta}\frac{(2-\varphi k-\varphi)^3}{g^{1/2}}\left(\frac{(\Gamma^{(2)}_{k,\varphi,b})^{1/2}}{v_{1,k}(D)}\right)^{3/2} \tag{D.7}$$

is satisfied with probability greater than $1-\delta$ as D varies, where $\Phi(\cdot)$ is the standard normal c.d.f.

Remark D.4. To the best of our knowledge, the only Stein's method central limit theorem in the Kolmogorov distance, applicable to our setting, is given in Zhang (2022), which generalizes the argument of Shao and Zhang (2019). In Appendix D.6, we show that this central limit theorem implies a bound that does not reduce as either g or k increase. ■

D.2 Reproducibility

We now characterize accuracy of the nominal reproducibility error of Algorithm 1.

Theorem D.4. *Suppose that the conditional variance $\mathrm{Var}(a(\mathsf{r}, D) \mid D)$ is strictly positive, almost surely, where r denotes a random collection drawn uniformly from $\mathcal{R}_{n,k,b}$. Suppose that the collections $\mathsf{R}_{\hat{g},k}$ and $\mathsf{R}'_{\hat{g}',k}$ are independently obtained using Algorithm 1. If Assumptions 4.1 and 4.2 hold, the data D are independent and identically distributed, and the eighth-order split stability $\zeta^{(8)}$ is finite, then, for all sufficiently small ξ, the inequality*

$$\begin{aligned} &P\left\{|a(\mathsf{R}_{\hat{g},k}, D)-a(\mathsf{R}'_{\hat{g}',k}, D)|\leq \xi \mid D\right\}-(1-\beta)\,| \\ &\quad\lesssim \left(\frac{\xi}{z_{1-\beta/2}}\frac{(2-\varphi k-\varphi)^4\Gamma^{(1)}_{k,\varphi,b}(\Gamma^{(2)}_{k,\varphi,b})^{1/2}}{\delta^{3/2}(v_{1,k}\left(D\right))^{5/2}}\right)^{1/2} \\ &\qquad\cdot\log^{3/4}\left(\frac{z_{1-\beta/2}}{\xi}\frac{\delta(v_{1,k}(D))^2}{(2-\varphi k-\varphi)^3(\Gamma^{(2)}_{k,\varphi,b})^{3/4}}\right), \end{aligned} \tag{D.8}$$

holds with probability greater than $1-\delta$ as D varies.

Remark D.5. Recall the definition of the oracle stopping time $g^\star$ given in (3.7). The bound (D.17) is obtained by decomposing the reproducibility error into two terms. The first term involves the error in a normal approximation to the difference $a(\mathsf{R}_{g^\star,k}, D)-a(\mathsf{R}'_{g^\star,k}, D)$. As $g^\star$ is deterministic

conditional on D, a bound on this term follows from an argument very similar to the proof of Theorem D.3. The second term involves the differences $a(\mathsf{R}_{\hat{g},k}, D) - a(\mathsf{R}_{g^\star,k}, D)$ and $a(\mathsf{R}'_{\hat{g}',k}, D) - a(\mathsf{R}'_{g^\star,k}, D)$. The key step in bounding these quantities involves deriving a high probability bound for the difference $\hat{g} - g^\star$. This follows by combining a concentration inequality analogous to Theorem D.1 for the estimator $\hat{v}_{g,k}(D)$ with a maximal inequality due to Steiger (1970). ■

D.3 Specialization to Cross-Split, Sample-Stable Statistics

In this section, we specialize the results stated in Appendices D.1 and D.2 to cross-fit, sample-stable statistics. That is, we focus attention to the setting where $n = k \cdot b$ and impose Assumption 4.3. By doing this, we prove each of the results stated in Section 4.

We begin by stating the following corollary of Theorem D.1, which is referenced in Footnote 22.

Corollary D.1. *Suppose that Assumptions 4.1 to 4.3 hold, that the data D are independently and identically distributed, and that the statistic $a(\mathsf{R}_{1,k}, D)$ has a non-zero variance conditional on D almost surely. If the fourth-order split stability $\zeta^{(4)}$ is finite, then, for each $\varepsilon > 0$, the inequality*

$$P\left\{ \left| a(\mathsf{R}_{g,k}, D) - \overline{a}\,(D) \right| \leq \sqrt{\frac{b-1}{n^2}\frac{1}{g}\frac{\log(\varepsilon^{-1})}{\delta}} \mid D \right\} \geq 1 - \varepsilon \tag{D.9}$$

holds with probability greater than $1 - \delta$ as D varies.

Proof. Corollary D.1 follows immediately from Theorem D.1 by restricting attention to the case that $n = k \cdot b$ and applying Assumption 4.3. In particular, observe that if $n = k \cdot b$, then $\Gamma_{k,\varphi,b} = \sigma^{(2,b-1)}_{\mathsf{train}}$ and

$$(2 - \varphi k - \varphi)^2 = (1 - \varphi)^2 = \left(\frac{n-b}{b}\right)^2 . \tag{D.10}$$

Applying Assumption 4.3 then gives

$$\Gamma_{k,\varphi,b} = \sigma^{(2,b-1)}_{\mathsf{train}} \lesssim \left(\frac{\sqrt{b-1}}{n-b}\right)^2 . \tag{D.11}$$

Plugging (D.10) and (D.11) into Theorem D.1 gives the desired bound. ■

Next, we show that Theorem D.2 implies the following generalization of Theorem 4.1 to higher-order moments. Theorem 4.1 is a strictly weaker result, as it only holds for the second moment.

Corollary D.2. *Suppose that Assumptions 4.1 to 4.3 hold, the data D are independently and identically distributed, and $n = k \cdot b$. If the $4r$th-order split stability $\zeta^{(4)}$ is finite, then, for each $\delta > 0$, the inequality*

$$\mathbb{E}\left[\left(a\left(\mathsf{R}_{g,k}, D\right) - \overline{a}\left(D\right) \right)^{2r} \mid D \right] \lesssim \left(\frac{b-1}{n^2}\frac{1}{g} \right)^{r/2} \tag{D.12}$$

holds with probability greater than $1 - \delta$ as D varies.

Proof. If $n = k \cdot b$, then $\Gamma^{(r)}_{k,\varphi,b} = \sigma^{(2r,b-1)}_{\mathsf{valid}}$. Applying Assumption 4.3 then gives

$$\Gamma^{(r)}_{k,\varphi,b} \lesssim \left(\frac{\sqrt{b-1}}{n-b}\right)^{2r} . \tag{D.13}$$

Plugging (D.10) and (D.13) into (D.4) gives

$$\mathbb{E}\left[\left(a\left(\mathsf{R}_{g,k}, D\right) - \overline{a}\left(D\right)\right)^{2r}\right] \lesssim \left(\frac{1}{nkg}\right)^{r} , \tag{D.14}$$

where we omit constants the depend only on r. ■

In turn, we specialize the non-asymptotic central limit theorem Theorem D.3 cross-fit, sample-stable statistics. This result suggests that, although the aggregate statistic $a(\mathsf{R}_{g,k}, D)$ is more concentrated at larger values of k, the quality of a normal approximation to its conditional distribution does not necessarily improve. This result is referenced in Footnote 27.

Corollary D.3. *Suppose that Assumptions 4.1 to 4.3 hold, the data D are independently and identically distributed, $n = k \cdot b$, and the conditional variance $v_{1,k}(D) = \mathrm{Var}(a(\mathsf{r}, D) \mid D)$ is strictly positive almost surely, where r denotes a random collection drawn uniformly from $\mathcal{R}_{n,k,b}$. If the 8th-order split stability $\zeta^{(8)}$ is finite, then, for all g, the inequality*

$$\sup_{z\in\mathbb{R}} \left| P\left\{ \frac{a\left(\mathsf{R}_{g,k}, D\right) - \overline{a}\left(D\right)}{\sqrt{v_{g,k}\left(D\right)}} \leq z \mid D \right\} - \Phi(z) \right| \lesssim \frac{1}{\delta}\left(\frac{1}{n}\frac{1}{k}\frac{b-1}{v_{1,k}(D)}\right)^{3/2} \sqrt{\frac{1}{g}} \tag{D.15}$$

is satisfied with probability greater than $1-\delta$ as D varies, where $\Phi(\cdot)$ is the standard normal c.d.f.

Proof. As before, Corollary D.3 follows by restricting attention to the case that $n = k \cdot b$ and imposing Assumption 4.3. In particular, Corollary D.3 is obtained by plugging the bounds (D.10) and (D.13) into (D.7). ■

Remark D.6. In this case, the quantities g and k enter differently. In particular, observe that, by applying the variance bound (4.9) for the case $g = 1$, to lower bound the rate (D.15), we get

$$\left(\frac{1}{n}\frac{1}{k}\frac{1}{v_{1,k}(D)}\right)^{3/2} \sqrt{\frac{1}{g}} \gtrsim \sqrt{\frac{1}{g}} . \tag{D.16}$$

Written differently, Corollary D.3 suggests that the quality of a normal approximation to the conditional distribution of the aggregate statistic $a\left(\mathsf{R}_{g,k}, D\right)$ does not increase with k—it only depends on g. ■

Finally, we show that Theorem 4.2 is a corollary of Theorem D.4 by restricting attention to the case that $n = k \cdot b$ and applying Assumption 4.3. We restate Theorem 4.2 below as a corollary for ease of reference.

Corollary D.4. *Suppose that the collections $\mathsf{R}_{\hat{g},k}$ and $\mathsf{R}'_{\hat{g}',k}$ are independently obtained using Algorithm 1. If Assumptions 4.1 to 4.3 hold, the conditional variance $v_{1,k}(D) = \mathrm{Var}(a(\mathsf{r}, D) \mid D)$ is strictly positive, almost surely, the data D are independent and identically distributed, and the eighth-order split stability $\zeta^{(8)}$ is finite, then for all sufficiently small ξ, the inequality*

$$\left| P\left\{ \left| a(\mathsf{R}_{\hat{g},k}, D) - a(\mathsf{R}'_{\hat{g}',k}, D) \right| \geq \xi \mid D \right\} - \beta \right| \lesssim \frac{1}{\delta^{3/4}} \frac{1}{kn} \left(\frac{1}{v_{1,k}(D)} \right)^{5/4} \left(\frac{\xi}{z_{1-\beta/2}} \right)^{1/2}, \tag{D.17}$$

holds with probability greater than $1 - \delta$ as D varies, where in writing (D.17), we have omitted a multiplicative term that converges to zero logarithmically as ξ decreases to zero.

Proof. Observe that if $n = k \cdot b$, then the right-hand-side of the inequality (D.17) can be written

$$\left(\frac{\xi}{z_{1-\beta/2}} \frac{\sigma_{\mathsf{train}}^{(2,b-1)} (\sigma_{\mathsf{train}}^{(4,b-1)})^{1/2}}{\delta^{3/2} (v_{1,k}(D))^{5/2}} \left(\frac{n-b}{n} \right)^4 \right)^{1/2} \cdot \log^{3/4} \left(\frac{z_{1-\beta/2}}{\xi} \left(\frac{n}{n-b} \right)^3 \frac{\delta (v_{1,k}(D))^2}{(\sigma_{\mathsf{train}}^{(4,b-1)})^{3/4}} \right). \tag{D.18}$$

By applying Assumption 4.3, the non-logarithmic factor reduces to

$$\left(\frac{\xi}{z_{1-\beta/2}} \frac{1}{\delta^{3/2} (v_{1,k}(D))^{5/2}} \left(\frac{\sqrt{b-1}}{n} \right)^4 \right)^{1/2} \leq \left(\frac{1}{\delta^{3/2}} \frac{\xi}{z_{1-\beta/2}} \left(\frac{1}{kn} \right)^2 \left(\frac{1}{v_{1,k}(D)} \right)^{5/2} \right)^{1/2} \tag{D.19}$$

as required. ∎

D.4 Constructing a Stein Representer

Suppose that we are interested in studying the statistic $f(X)$, where X is random variable valued on the separable metric space $\mathcal{X}$. The method of exchangeable pairs has two ingredients. First, we need to construct a random variable X' such that (X, X') is an exchangeable pair. Second, we need to construct an antisymmetric function $F(X, X')$ such that

$$f(X) = \mathbb{E}[F(X, X') \mid X] \tag{D.20}$$

almost surely. We will refer to the function $F(X, X')$ as a "Stein representer" for $f(X)$.

In many applications, the Stein representer (D.20) induced by a suitable exchangeable pair (X, X') can be derived in closed form. See e.g Chen et al. (2011) and Ross (2011). A closed form derivation is more challenging in our setting, where the collection $\mathsf{R}_{g,k}$ takes the place of the random variable X. To address this issue, we apply a method due to Chatterjee (2005) for constructing Stein representers through a pair of coupled Markov chains induced by an appropriately chosen exchangeable pair.

Chatterjee's construction is founded on a observation, due to Stein (1986), that an exchangeable pair (X, X') induces a reversible Markov kernel K through

$$Kg(x) = \mathbb{E}\left[g(X') \mid X = x\right] ,$$

where g is any function satisfying $\mathbb{E}\left[|g(X)|\right] < \infty$. Suppose that $\{X_m\}_{m\geq 0}$ and $\{X'_m\}_{m\geq 0}$ are two Markov chains constructed with the kernel induced by (X, X') and coupled in such a way that the marginal distributions of X_m and X'_m depend only on the initial conditions X_0 and X'_0, respectively. Chatterjee makes the following observation. If there exists a constant C such that

$$\sum_{m=0}^{\infty} \left|\mathbb{E}\left[f(X_m) - f(X'_m) \mid X_0 = x, X'_0 = y\right]\right| \leq C , \tag{D.21}$$

for each x and y in $\mathcal{X}$, then the function

$$F(x, y) = \sum_{m=0}^{\infty} \mathbb{E}\left[f(X_m) - f(X'_m) \mid X_0 = x, X'_0 = y\right]$$

is a Stein representer for $f\left(X\right)$. See Paulin et al. (2013, 2016) for applications of this idea to the derivation of matrix concentration inequalities. To apply this construction to our setting, we have two tasks. First, we need to specify a suitable exchangeable pair. Second, we need to construct a pair of coupled Markov chains induced by this pair that satisfy the finiteness condition (D.21). Throughout, for a vector $x = (x_i)_{i=1}^n$ we let $(x_{-\ell}, y)$ denote the vector formed by replacing the ℓth component of x with y.

Our construction is premised on the observation that the random collection of splits $\mathsf{R}_{g,k}$ can be generated by a random collection of permutations. To see this, let $\mathcal{P}_n$ denote the set of permutations of the set $[n]$, treating each $\pi \in \mathcal{P}_n$ as a bijection from $[n]$ to $[n]$. Observe that each permutation $\pi \in \mathcal{P}_n$ can be associated with an element of $\mathcal{R}_{n,k,b}$, denoted by $\mathsf{r}_k\left(\pi\right) = \left(\mathsf{s}_1\left(\pi\right), \ldots, \mathsf{s}_k\left(\pi\right)\right)$, through

$$\mathsf{s}_i\left(\pi\right) = \left\{\pi\left(k \cdot (i-1) + 1\right), \ldots, \pi\left(k \cdot (i-1) + b\right)\right\} .$$

If $\boldsymbol{\pi} = (\pi_i)_{i=1}^g$denotes a collection of permutations drawn independently and uniformly at random from $\mathcal{P}_n$, then the collection $\mathsf{R}_{g,k}\left(\boldsymbol{\pi}\right) = \left(\mathsf{r}_k\left(\pi_i\right)\right)_{i=1}^g$ is equidistributed with the collection $\mathsf{R}_{g,k}$ defined in Section 2.

Now, we construct an exchangeable pair $(\boldsymbol{\pi}, \boldsymbol{\pi}')$, keeping in mind that our aim is to verify a condition of the form (D.21). For any permutation $\pi \in \mathcal{P}_n$ and indices $i, j \in [n]$, define the updated permutation

$$\hat{\pi}\left(i, j\right)\left(x\right) = \begin{cases} j, & x = i, \\ \pi\left(i\right), & x = \pi^{-1}\left(j\right), \\ \pi\left(x\right), & \text{otherwise.} \end{cases}$$

In other words, $\hat{\pi}(i,j)$ is identical to π, except that i maps to j and $\pi^{-1}(j)$ maps to $\pi(i)$. Let L be distributed uniformly on $[g]$ and let I and J be independently and uniformly distributed on $[n]$. Define the modified collection

$$\boldsymbol{\pi}' = (\pi_{-L}, \hat{\pi}_L(I,J)).$$

and observe that $(\boldsymbol{\pi}, \boldsymbol{\pi}')$ is an exchangeable pair.

With the exchangeable pair $(\boldsymbol{\pi}, \boldsymbol{\pi}')$ in place, we choose a coupled pair of Markov chains that it induces. For each $m \geq 1$, let L_m be distributed uniformly on $[g]$ and let I_m and J_m be distributed uniformly on $[n]$. Construct $(\boldsymbol{\pi}_m, \boldsymbol{\pi}'_m)$ from the pair $(\boldsymbol{\pi}_0, \boldsymbol{\pi}'_0) = (\boldsymbol{\pi}, \boldsymbol{\pi}')$ by setting

$$\boldsymbol{\pi}_m = (\pi_{m-1,-L_m}, \hat{\pi}_{m-1,L_m}(I_m, J_m)) \quad \text{and} \quad \boldsymbol{\pi}'_m = (\pi'_{m-1,-L_m}, \hat{\pi}'_{m-1,L_m}(I_m, J_m)) \tag{D.22}$$

recursively. In other words, the Markov chain $\boldsymbol{\pi}'_0$ is initialized by choosing one permutation in $\boldsymbol{\pi}_0$ and swapping one pair of indices. In the mth iteration of the Markov chain $(\boldsymbol{\pi}_m, \boldsymbol{\pi}'_m)_{m\geq 0}$, the permutations π_{m-1,L_m} and π'_{m-1,L_m} are selected and updated so that I_m now maps to J_m. As the iterations proceed, I_m will continue to map to the same index in the L_mth permutation in both collections. That is, in each iteration that a new permutation L and index I are selected, the two collections become more similar. Eventually, every L and I will have been selected, the two collections $\boldsymbol{\pi}_m$ and $\boldsymbol{\pi}'_m$ will be the same, and so $a(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D) - a(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D) = 0$. This will imply the finiteness (D.21). This argument is formalized in the proof of the following Lemma.

Lemma D.1. *The function*

$$A(\boldsymbol{\pi}, \boldsymbol{\pi}' \mid D) = \sum_{m=0}^{\infty} \mathbb{E}\left[\left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right)\right) \mid \boldsymbol{\pi}_0 = \boldsymbol{\pi}, \boldsymbol{\pi}'_0 = \boldsymbol{\pi}', D\right],$$

is finite, antisymmetric, and satisfies the equality

$$\mathbb{E}\left[A(\boldsymbol{\pi}, \boldsymbol{\pi}' \mid D) \mid \boldsymbol{\pi}, D\right] = a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}(D) \tag{D.23}$$

almost surely.

D.5 Proofs

D.5.1 Proofs for Non-Sequential Results. To obtain the concentration inequality Theorem D.1 and Burkholder-Davis-Gundy inequality Theorem D.2, we apply the following result due to Chatterjee (2005, 2007), which we have augmented to be applicable under a set of assumptions considered in Paulin et al. (2016).

Lemma D.2. *Let $\mathcal{X}$ be a separable metric space and suppose that (X, X') is an exchangeable pair of $\mathcal{X}$-valued random variables. Let $f : \mathcal{X} \to \mathbb{R}$ be a square integrable function and let $F : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$*

be a Stein representer for f. For each positive integer (r), define the quantities

$$U_f^{(r)}(X) = \frac{1}{2}\mathbb{E}\left[(f(X) - f(X'))^{2r} \mid X\right] \quad \textit{and} \quad U_F^{(r)}(X) = \frac{1}{2}\mathbb{E}\left[F(X, X')^{2r} \mid X\right]. \tag{D.24}$$

If there exist nonnegative constants u and s such that

$$U_f^{(1)}(X) \leq s^{-1}u \quad \textit{and} \quad U_F^{(1)}(X) \leq su, \tag{D.25}$$

then the concentration inequality

$$P\{|f(X)| \geq \delta\} \leq 2\exp\left(-t^2/2u\right) \tag{D.26}$$

holds for all $t \geq 0$. Moreover, the moment inequality

$$\mathbb{E}\left[f(X)^{2r}\right] \leq (2r-1)^r \left(s\mathbb{E}\left[U_F^{(r)}(X)\right] + s^{-1}\mathbb{E}\left[U_f^{(r)}(X)\right]\right) \tag{D.27}$$

holds for all positive integers r for any positive constant s.

Throughout, to ease notation, we use the short hand

$$Z = (\mathsf{R}_{g,k}(\boldsymbol{\pi}), D) \quad \text{and} \quad Z' = (\mathsf{R}_{g,k}(\boldsymbol{\pi}'), D).$$

The Markov chains $(Z_m)_{m\geq 0}$ and $(Z'_m)_{m\geq 0}$ are defined accordingly and we simplify $A(\boldsymbol{\pi}, \boldsymbol{\pi}' \mid D)$ to $A(Z, Z')$. To apply Lemma D.2, we are required to develop bounds for the objects

$$U_a^{(r)}(Z) = \frac{1}{2}\mathbb{E}\left[(a(Z) - a(Z'))^{2r} \mid Z\right] \quad \text{and} \quad U_A^{(r)}(Z) = \frac{1}{2}\mathbb{E}\left[A(Z, Z')^{2r} \mid Z\right].$$

Our approach is based on the following Lemma, which combines a generalization of an idea due to Lemma 10.4 of Paulin et al. (2016) with a Markov type bound.

Lemma D.3. *Let $r = 2^c$ for some positive integer c. Let $f : \mathcal{Z} \to \mathbb{R}$ be a function such that there exists a square integrable random variable W with*

$$\left(\sum_{m=0}^{\infty} \mathbb{E}\left[f(Z_m) - f(Z'_m) \mid Z_0 = Z, Z'_0 = Z'\right]\right)^r \leq W \tag{D.28}$$

almost surely. If the inequality

$$\mathbb{E}\left[\mathbb{E}\left[f(Z_m) - f(Z'_m) \mid Z_0 = Z, Z'_0 = Z'\right]^r \mid \boldsymbol{\pi}\right] \leq h_m^r \tag{D.29}$$

holds for each $m \geq 0$ and each collection $\boldsymbol{\pi}$, where $(h_m)_{m\geq 0}$ is a deterministic sequence of nonnegative numbers, then the inequalities

$$\frac{1}{2}\mathbb{E}\left[(f(Z) - f(Z'))^r \mid Z\right] \leq \frac{h_0^r}{\delta} \quad \textit{and} \tag{D.30}$$

$$\frac{1}{2}\mathbb{E}\left[\left(\sum_{m=0}^{\infty} \mathbb{E}\left[f(Z_m) - f(Z'_m) \mid Z_0 = Z, Z'_0 = Z'\right]\right)^r \mid Z\right] \leq \frac{1}{\delta}\left(\sum_{m=0}^{\infty} h_m\right)^r \tag{D.31}$$

both hold with probability greater than $1-\delta$ *as* D *varies*

To apply this Lemma, we begin by noting that the inequality

$$\begin{aligned}&\left(\sum_{m=0}^{\infty}\mathbb{E}\left[a\left(Z_m\right)-a\left(Z_m'\right)\mid Z_0=Z,Z_0'=Z'\right]\right)^2\\&\lesssim g^2n^4\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left(T\left(\mathsf{s},U,D\right)-T\left(\mathsf{s}',U,D\right)\right)^2\end{aligned}\tag{D.32}$$

follows from Lemma E.1, stated in Appendix E.1. Moreover, the right hand side of (D.32) is square integrable, as the fourth order split-stability $\zeta^{(4)}$ is finite by assumption. Deterministic bounds of the form (D.29) are obtained through the following Lemma.

Lemma D.4. *Under Assumptions 4.1 and 4.2, for all integers* $m\geq 0$ *and* $r\geq 1$*, the inequality*

$$\begin{aligned}&\mathbb{E}\left[\mathbb{E}\left[a(Z_m)-a(Z_m')\mid Z_0=Z,Z_0'=Z'\right]^{2r}\mid\boldsymbol{\pi}\right]\\&\leq 2^{4r}\left(1-\frac{2}{gn^2}\right)^{2mr}\left(\frac{2n-bk-b}{gn^2}\right)^{2r}\Gamma_{k,\varphi,b}^{(r)}\end{aligned}$$

holds almost surely, where $\Gamma_{k,\varphi,b}^{(r)}$ *is defined in the statement of Theorem D.2.*

Combining Lemmas D.3 and D.4, we have that

$$U_A^{(r)}(Z)\leq\frac{1}{\delta}\left(\frac{gn^2}{2}\right)^r\left(\frac{2^4\left(2n-bk-b\right)^2}{gn^2}\right)^r\Gamma_{k,\varphi,b}^{(r)}$$

and

$$U_a^{(r)}(Z)\leq\frac{1}{\delta}\left(\frac{2}{gn^2}\right)^r\left(\frac{2^4\left(2n-bk-b\right)^2}{gn^2}\right)^r\Gamma_{k,\varphi,b}^{(r)}$$

with probability $1-\delta$. Corollary D.1 is obtained by setting $r=1$ and applying (D.26) of Lemma D.2 with $s=gn^2/2$ and

$$u=\frac{1}{\delta}\frac{2^4\left(2n-bk-b\right)^2}{gn^2}\Gamma_{n,k,b}^{(1)}.$$

Similarly, Theorem D.2 is obtained by applying (D.27) of Lemma D.2 with $s=(gn^2/2)^r$.

The normal approximation error bound Theorem D.3 follows from Theorem D.2. To see this, consider the centered statistic

$$a\left(Z\right)-\overline{a}\left(D\right)=\frac{1}{g}\sum_{\ell=1}^{g}\overline{a}\left(\mathsf{r}_\ell,D\right),\quad\text{where}\quad\overline{a}\left(\mathsf{r}_\ell,D\right)=\frac{1}{k}\sum_{i=1}^{k}\left(T(\mathsf{s}_{\ell,i},D)-\overline{a}\left(D\right)\right)\tag{D.33}$$

for each ℓ in $[g]$. Conditional on the data D, the statistics $\overline{a}\left(\mathsf{r}_\ell,D\right)$ are independent, identically distributed, and mean zero. Moreover, we have that

$$\mathbb{E}\left[\left|\overline{a}\left(\mathsf{r}_\ell,D\right)\right|^3\right]\leq 3^2 2^6\left(2-\varphi k-\varphi\right)^3\left(\Gamma_{k,\varphi,b}^{(2)}\right)^{3/4}\tag{D.34}$$

by Hölder's inequality and Theorem D.2. Hence, we find that

$$\frac{\mathbb{E}\left[|\overline{a}\left(\mathsf{r}_{\ell}, D\right)|^{3} \mid D\right]}{g^{1/2}\left(v_{1,k}(D)\right)^{3/2}} \leq \frac{3^{2} 2^{6}}{\delta} \frac{(2-\varphi k-\varphi)^{3}}{\left(v_{1,k}(D)\right)^{3/2}} \frac{\left(\Gamma_{k,\varphi,b}^{(2)}\right)^{3/4}}{g^{1/2}}$$

holds with probability greater than $1-\delta$, by combining (D.34) with the Markov inequality. The proof then follows by the Berry-Esseen inequality. See e.g., Corollary 1 of Shevtsova (2011). ■

D.5.2 Proofs for Sequential Results. The first step for verifying Theorem D.4 is deriving a large deviation bound for the variance estimator $\hat{v}\left(\mathsf{R}_{g,k}, D\right)$ defined in (3.4). This is obtained in the following Lemma, which follows from an argument very similar to the proof of Theorem D.1.

Lemma D.5. *Suppose that Assumptions 4.1 and 4.2 hold and that the data D are independent and identically distributed. If the eighth-order split-stability $\zeta^{(8)}$ is finite, then the conditional concentration inequality*

$$\log \frac{1}{4} P\left\{\left|\frac{\hat{v}(\mathsf{R}_{g,k}, D)}{v_{g,k}\left(D\right)}-1\right| \geq t \mid D\right\} \lesssim -\frac{\delta\left(v_{1,k}(D)\right)^{2}}{(2-\varphi k-\varphi)^{4}} \frac{g t^{2}}{\Gamma_{k,\varphi,b}^{(2)}}$$

holds for all $t>0$ with probability greater than $1-\delta$ as D varies.

We focus our analysis on the error

$$|P\left\{a(\mathsf{R}_{\hat{g},k}, D)-a(\mathsf{R}_{\hat{g}',k}', D) \leq \xi \mid D\right\}-(1-\beta/2)|. \tag{D.35}$$

An analogous argument will yield the same bound for the lower tail. We begin by bounding (D.35) with quantities that will be easier to handle in isolation. Define the objects

$$U\left(\mathsf{R}_{g,k}, D\right)=\frac{1}{g^{\star}}\left(\sum_{i=1}^{g} \overline{a}\left(\mathsf{r}_{i,k}, D\right)-\sum_{i=1}^{g^{\star}} \overline{a}\left(\mathsf{r}_{i,k}, D\right)\right) \quad \text{and} \tag{D.36}$$

$$Q\left(\mathsf{R}_{g,k}, D\right)=\left(1-\frac{g}{g^{\star}}\right)\left(a(\mathsf{R}_{g,k}, D)-\overline{a}\left(D\right)\right) . \tag{D.37}$$

The following Lemma bounds the error (D.35) in terms of the error in the normal approximation to the quantity $a(\mathsf{R}_{g^{\star},k}, D)-a(\mathsf{R}_{g^{\star},k}', D)$ and generic high probability bounds on (D.36) and (D.37).

Lemma D.6. *Define the events*

$$\mathcal{U}_{k,\lambda}\left(D\right)=\left\{|U(\mathsf{R}_{\hat{g},k}, D)-U(\mathsf{R}_{\hat{g}',k}', D)| \leq \lambda \sqrt{2 v_{g^{\star},k}\left(D\right)}\right\} \quad \textit{and}$$

$$\mathcal{Q}_{k,\lambda}(D)=\left\{\left|Q(\mathsf{R}_{g,k}, D)-Q(\mathsf{R}_{\hat{g}',k}', D)\right| \leq \lambda \sqrt{2 v_{g^{\star},k}\left(D\right)}\right\}.$$

The quantity (D.35) *is bounded above by*

$$\sup_{z\in\mathbb{R}}\left|P\left\{\frac{a(\mathsf{R}_{g^\star,k},D)-a(\mathsf{R}'_{g^\star,k},D)}{\sqrt{2v_{g^\star,k}(D)}}\le z\mid D\right\}-\Phi(z)\right| + 2\lambda+\left(1-P\left\{\mathcal{U}_{k,\lambda}(D)\cap\mathcal{Q}_{k,\lambda}(D)\mid D\right\}\right), \tag{D.38}$$

where $\Phi(\cdot)$ *is the standard normal c.d.f.*

Thus, it remains to give suitable bounds for the objects in (D.38). We state these bounds in terms of the quantities

$$\rho_{k,\varphi,b}(\xi,\beta\mid D)=\frac{\xi}{z_{1-\beta/2}}\frac{(2-\varphi k-\varphi)^3(\Gamma^{(2)}_{k,\varphi,b})^{3/4}}{\delta\left(v_{1,k}(D)\right)^2} \quad \text{and} \tag{D.39}$$

$$\lambda_{k,\varphi,b}(\xi,\beta\mid D)=\left(\frac{\xi}{z_{1-\beta/2}}\frac{(2-\varphi k-\varphi)^4\Gamma^{(1)}_{k,\varphi,b}(\Gamma^{(2)}_{k,\varphi,b})^{1/2}}{\delta^{3/2}(v_{1,k}(D))^{5/2}}\right)^{1/2}, \tag{D.40}$$

respectively. Each part of following Lemma follows from an application of Lemma D.6.

Lemma D.7. *Suppose that Assumptions 4.1 and 4.2 hold, that the data* D *are independent and identically distributed, that the conditional variance* $v_{1,k}(D)=\mathrm{Var}(a(\mathsf{r},D)\mid D)$ *is strictly positive almost surely, and that the eighth-order split stability* $\zeta^{(8)}$ *is finite.*

(i) *The inequality*

$$\left|P\left\{\frac{a(\mathsf{R}_{g^\star,k},D)-a(\mathsf{R}'_{g^\star,k},D)}{\sqrt{2v_{g^\star,k}(D)}}\le z\mid D\right\}-\Phi(z)\right|\lesssim\rho_{k,\varphi,b}(\xi,\beta\mid D)$$

is satisfied with probability greater than $1-\delta$ *as* D *varies.*

(ii) *The conditional concentration inequality*

$$P\left\{\frac{|U(\mathsf{R}_{\hat{g},k},D)-U(\mathsf{R}'_{\hat{g}',k},D)|}{\sqrt{2v_{g^\star,k}(D)}}\ge\lambda_{k,\varphi,b}(\xi,\beta\mid D)\log^{3/4}\left(\rho_{k,\varphi,b}(\xi,\beta\mid D)^{-1}\right)\mid D\right\} \lesssim\rho_{k,\varphi,b}(\xi,\beta\mid D)$$

holds with probability greater than $1-\delta$ *as* D *varies.*

(iii) *For all sufficiently small* ξ*, the conditional concentration inequality*

$$P\left\{\frac{|Q(\mathsf{R}_{\hat{g},k},D)-Q(\mathsf{R}'_{\hat{g}',k},D)|}{\sqrt{2v_{g^\star,k}(D)}}\ge\lambda_{k,\varphi,b}(\xi,\beta\mid D)\right\}\lesssim\rho_{k,\varphi,b}(\xi,\beta\mid D)$$

holds with probability greater than $1-\delta$ *as* D *varies.*

Now, observe that $\rho_{k,\varphi,b}(\xi, \beta \mid D)$ is smaller than $\lambda_{k,\varphi,b}(\xi, \beta \mid D)$ for all sufficiently small ξ, almost surely. Consequently, by combining Lemma D.6 and Lemma D.7, we find that

$$\begin{aligned} &|P\left\{|a(\mathsf{R}_{\hat{g},k}, D) - a(\mathsf{R}'_{\hat{g}',k}, D)| \leq \xi \mid D\right\} - (1-\beta)| \\ &\qquad \lesssim \left(\frac{\xi}{z_{1-\beta/2}} \frac{(2-\varphi k-\varphi)^4 \Gamma^{(1)}_{k,\varphi,b} (\Gamma^{(2)}_{k,\varphi,b})^{1/2}}{\delta^{3/2} (v_{1,k}(D))^{5/2}}\right)^{1/2} \\ &\qquad\qquad \cdot \log^{3/4}\left(\frac{z_{1-\beta/2}}{\xi} \frac{\delta (v_{1,k}(D))^2}{(2-\varphi k-\varphi)^3 (\Gamma^{(2)}_{k,\varphi,b})^{3/4}}\right) \end{aligned} \tag{D.41}$$

with probability greater than $1-\delta$, as required. ■

D.6 Comparison with Zhang (2022)

We state a Berry-Esseen bound for $a(\mathsf{R}_{g,k}, D)$ through an application of a result due to Zhang (2022). In contrast to the bound stated in Theorem D.3, the bound obtained here does not shrink as g increases. On the other hand, the bound obtained below is unconditional. It is straightforward to modify our argument to give an analogous high-probability conditional bound.

Theorem D.5. *Let W denote a standard normal random variable. Suppose that Assumptions 4.1 and 4.2 hold and that the data D are independent and identically distributed. If the eighth-order split stability $\zeta^{(8)}$ is finite, then the Berry-Esseen inequality*

$$d_K\left(\frac{a(\mathsf{R}_{g,k}, D) - \overline{a}(D)}{\sqrt{\mathbb{E}[v_{g,k}(D)]}}, W\right) \leq \frac{4(2-\varphi k-\varphi)^2 (\Gamma^{(2)}_{k,\varphi,b})^{1/2}}{\mathbb{E}[v_{1,k}(D)]}$$

is satisfied.

D.6.1 Proof of Theorem D.5. We apply the following central limit theorem, due to Zhang (2022). This result generalizes Theorem 2.1 of Shao and Zhang (2019) to accommodate general Stein representers.

Theorem D.6 (Theorem 4.1, Zhang, 2022)**.** *Let $\mathcal{X}$ be a separable metric space and suppose that (X, X') is an exchangeable pair of $\mathcal{X}$-valued random variables. Suppose that $f : \mathcal{X} \to \mathbb{R}$ and $F : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ are square-integrable functions such that F is antisymmetric and*

$$\mathbb{E}[F(X, X') \mid X] = f(X)$$

almost surely. Assume that $\mathrm{Var}(f(X))$ is finite and non-zero and that $\mathbb{E}[f(X)] = 0$. Define the objects

$$\overline{f}(X) = f(X) / \sqrt{\mathrm{Var}(f(X))}. \tag{D.42}$$

$$G(X) = \frac{1}{2}\mathbb{E}[(f(X) - f(X'))F(X, X') \mid X] \quad \text{and} \tag{D.43}$$

$$\overline{G}(X) = \frac{1}{2}\mathbb{E}\left[\left(f(X) - f(X')\right)\left|F(X,X')\right| \mid X\right]. \tag{D.44}$$

Let W denote a standard normal random variable. The bound

$$d_K\left(\overline{f}(X), W\right) \leq \frac{\mathbb{E}\left[\left|G(X) - \mathbb{E}\left[G(X)\right]\right|\right] + \mathbb{E}\left[\left|\overline{G}(X)\right|\right]}{\mathrm{Var}\left(f(X)\right)} \tag{D.45}$$

is satisfied.

To this end, define the objects

$$B(Z) = \frac{1}{2}\mathbb{E}\left[\left(a(Z) - a(Z')\right)A(Z,Z') \mid Z\right] \quad \text{and}$$
$$\overline{B}(Z) = \frac{1}{2}\mathbb{E}\left[\left(a(Z) - a(Z')\right)\left|A(Z,Z')\right| \mid Z\right].$$

It will suffice to bound the quantity

$$\frac{\mathbb{E}\left[\left|B(Z) - \mathbb{E}\left[B(Z)\right]\right|\right] + \mathbb{E}\left[\left|\overline{B}(Z)\right|\right]}{\mathrm{Var}\left(a(Z) - \overline{a}(Z)\right)}. \tag{D.46}$$

Observe that

$$\mathbb{E}\left[\left|B(X) - \mathbb{E}\left[B(X)\right]\right|\right] \leq \sqrt{\mathrm{Var}\left(B(Z)\right)} \quad \text{and}$$
$$\mathbb{E}\left[\left|\overline{B}(Z)\right|\right] \leq \sqrt{\mathrm{Var}\left(\overline{B}(Z)\right)}$$

by the Cauchy-Schwarz inequality and the fact that $\mathbb{E}\left[\overline{B}(X)\right] = 0$ by exchangeability. Consequently, as

$$\mathrm{Var}\left(B(Z)\right) \leq \mathbb{E}\left[B(Z)^2\right] = \mathbb{E}\left[\left(a(Z) - a(Z')\right)^2 A(Z,Z')^2\right] = \mathrm{Var}\left(\overline{B}(Z)\right)$$

it will suffice to bound

$$2\mathbb{E}\left[\left(a(Z) - a(Z')\right)^2 A(Z,Z')^2\right]. \tag{D.47}$$

By Young's inequality, we have that

$$\mathbb{E}\left[\left(a(Z) - a(Z')\right)^2 A(Z,Z')^2\right] \leq \frac{1}{2}\left(s^{-1}\mathbb{E}\left[U_a^{(2)}(Z)\right] + s\mathbb{E}\left[U_A^{(2)}(Z)\right]\right),$$

where $U_a^{(2)}(Z)$ and $U_A^{(2)}(Z)$ are defined in Appendix D.5.1.

Observe that the bound

$$\left(\sum_{m=0}^{\infty}\mathbb{E}\left[a(Z_m) - a(Z_m') \mid Z_0 = Z, Z_0' = Z'\right]\right)^4$$
$$\leq \left(2gn^2 \max_{\mathsf{s},\mathsf{s}' \in \mathsf{S}_{n,b}}\left(T(\mathsf{s},D) - T(\mathsf{s}',D)\right)\right)^4 \tag{D.48}$$

holds by Lemma E.1 and that the right-hand side of (D.48) is square-integrable as the eighth-order split stability $\zeta^{(8)}$ is finite. Thus, by combining Lemma E.3 and Lemma D.4, we have that

$$\overline{U}_A^{(2)} \leq \left(\frac{gn^2}{2}\right)^2 \left(\frac{4\left(2n-bk-b\right)^2}{gn^2}\right)^2 \Gamma_{k,\varphi,b}^{(2)}$$

and

$$\overline{U}_a^{(2)} \leq \left(\frac{2}{gn^2}\right)^2 \left(\frac{4\left(2n-bk-b\right)^2}{gn^2}\right)^2 \Gamma_{k,\varphi,b}^{(2)}\,.$$

Hence, by taking $s = \left(gn^2/2\right)^2$, we find that (D.47) is bounded above by

$$\frac{4}{gn^2}\left(\left(2n-bk-b\right)^2 \left(\Gamma_{k,\varphi,b}^{(2)}\right)^{1/2}\right)$$

Now, we have that

$$\operatorname{Var}\left(a\left(Z\right)-\overline{a}\left(D\right)\right) = \mathbb{E}\left[v_{g,k}\left(D\right)\right]$$

by the law of total variance and the fact that $\mathbb{E}\left[a\left(Z\right)-\overline{a}\left(D\right) \mid D\right] = 0$. Consequently we can decompose

$$\mathbb{E}\left[v_{g,k}\left(D\right)\right] = \frac{\mathbb{E}[\phi_{n,b}(D)] + (k-1)\,\mathbb{E}[\gamma_{n,b}(D)]}{kg}. \tag{D.49}$$

Hence, we have that (D.46) is bounded above by

$$\frac{4\left(2-\varphi k-\varphi\right)^2 \left(\Gamma_{k,\varphi,b}^{(2)}\right)^{1/2}}{\mathbb{E}\left[v_{1,k}(D)\right]},$$

as required. ■

Appendix E. Proofs for Lemmas Stated in Appendix D

E.1 Proof of Lemma D.1

We use the following Lemma in several places.

Lemma E.1. *Let $\boldsymbol{\psi}$ and $\boldsymbol{\psi}'$ be two sets, each containing g elements of $\mathcal{P}_n$. The inequality*

$$\begin{aligned}&\sum_{m=0}^{\infty}\left|\mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m)\right)-a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m)\right) \mid \boldsymbol{\pi}_0=\boldsymbol{\psi},\boldsymbol{\pi}'_0=\boldsymbol{\psi}',D\right]\right|\\ &\leq 2gn^2 \max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left(T\left(\mathsf{s},D\right)-T\left(\mathsf{s}',D\right)\right)\end{aligned}$$

holds almost surely.

Observe that the quantity

$$\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left(T\left(\mathsf{s},D\right)-T\left(\mathsf{s}',D\right)\right)$$

is finite almost surely. Thus, the convergence of the series defining $A(\boldsymbol{\pi}, \boldsymbol{\pi}' \mid D)$ follows from Lemma E.1. Define the operator

$$\begin{aligned} K : \mathcal{F} &\to \mathcal{F} \\ f(\cdot) &\mapsto \mathbb{E}\left[f(\boldsymbol{\pi}') \mid \boldsymbol{\pi} = \cdot\right], \end{aligned}$$

where $\mathcal{F}$ is the set of all measurable functions supported on the domain of $\boldsymbol{\pi}$. Observe that

$$\begin{aligned} &\mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right) \mid \boldsymbol{\pi}_0 = \boldsymbol{\pi}, \boldsymbol{\pi}'_0 = \boldsymbol{\pi}', D\right] \\ &= \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - \overline{a}(D) \mid \boldsymbol{\pi}_0 = \boldsymbol{\pi}, D\right] - \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right) - \overline{a}(D) \mid \boldsymbol{\pi}'_0 = \boldsymbol{\pi}', D\right] \\ &= K^m\left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi})\right) - \overline{a}(D)\right) - K^{m+1}\left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}')\right) - \overline{a}(D)\right). \end{aligned}$$

Thus, for any m', we have that

$$\begin{aligned} &\sum_{m=0}^{m'} \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right) \mid \boldsymbol{\pi}_0 = \boldsymbol{\pi}, \boldsymbol{\pi}'_0 = \boldsymbol{\pi}', D\right] \\ &= a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right) - K^{m'+1}\left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right)\right). \end{aligned} \tag{E.1}$$

By Lemma E.1, the partial sums (E.1) converge almost everywhere and so the sequence

$$\left(K^{m+1}\left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right)\right)\right)_{m \geq 0} \tag{E.2}$$

also converges almost everywhere. Lemma E.1 also implies that the limit of (E.2) depends only on D, as

$$K^m\left(a\left(\left(\mathsf{R}_{g,k}\left(\boldsymbol{\psi}\right), D\right)\right) - \overline{a}\left(D\right)\right) - K^m a\left(\left(\mathsf{R}_{g,k}\left(\boldsymbol{\psi}'\right), D\right) - \overline{a}\left(D\right)\right) \to 0$$

for any $\boldsymbol{\psi}$ and $\boldsymbol{\psi}'$ each containing g elements of $\mathcal{P}_n$. Therefore, we have that

$$\begin{aligned} &\mathbb{E}\left[A\left(\boldsymbol{\pi}, \boldsymbol{\pi}' \mid D\right) \mid D\right] \\ &= \mathbb{E}\left[\lim_{n \to \infty} \left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right) - K^{m+1} a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right)\right) \mid D\right] \\ &= \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right) \mid D\right] - b\left(D\right), \end{aligned}$$

for some quantity

$$b\left(D\right) = \lim_{m \to \infty} K^m\left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right)\right)$$

that depends only on D. Observe that

$$\begin{aligned} &\mathbb{E}\left[A\left(\boldsymbol{\pi}, \boldsymbol{\pi}' \mid D\right) \mid D\right] \\ &= \mathbb{E}\left[\lim_{m' \to \infty} \sum_{m=0}^{m'} \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right) \mid \boldsymbol{\pi}_0 = \boldsymbol{\pi}, \boldsymbol{\pi}'_0 = \boldsymbol{\pi}', D\right] \mid D\right] \end{aligned}$$

$$= \lim_{m' \to \infty} \sum_{m=0}^{m'} \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right) \mid D\right] \qquad \text{(Dominated Conv.)}$$

$$= 0, \qquad \text{(Exchangeability)}$$

where the applicability of the Dominated Convergence Theorem follows from Lemma E.1. Thus, as

$$\mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right) \mid D\right] = 0,$$

we can conclude that $b\left(D\right) = 0$ almost surely. Hence, we find that

$$\begin{aligned}
&\mathbb{E}\left[A\left(\boldsymbol{\pi}, \boldsymbol{\pi}' \mid D\right) \mid \boldsymbol{\pi}, D\right] \\
&= \mathbb{E}\left[\lim_{m' \to \infty} \sum_{m=0}^{m'} \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right) \mid \boldsymbol{\pi}_0 = \boldsymbol{\pi}, \boldsymbol{\pi}'_0 = \boldsymbol{\pi}', D\right] \mid \boldsymbol{\pi}, D\right] \\
&= \lim_{m' \to \infty} \sum_{m=0}^{m'} \mathbb{E}\left[a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D\right) - a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D\right) \mid \boldsymbol{\pi}_0 = \boldsymbol{\pi}, \boldsymbol{\pi}'_0 = \boldsymbol{\pi}', D\right] \quad \text{(Dominated Conv.)} \\
&- \lim_{m' \to \infty} K^{m'+1}\left(a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right)\right) \\
&= a\left(\mathsf{R}_{g,k}(\boldsymbol{\pi}), D\right) - \overline{a}\left(D\right),
\end{aligned}$$

completing the proof. ■

E.2 Proof of Lemma D.2

First, observe that

$$U_F\left(X\right) \geq \frac{1}{2}\left(\mathbb{E}\left[F\left(X, X'\right) \mid X\right]\right)^2 = \frac{1}{2} f\left(X\right)^2,$$

where the inequality follows from Jensen's inequality and the definition of the Stein representer F. By (D.30), we have that

$$su \geq \frac{1}{2} f\left(X\right)^2.$$

Hence, the random variable $f\left(X\right)$ is bounded almost surely.

Now, suppose $h : \mathcal{X} \to \mathbb{R}$ is any measurable function such that $\mathbb{E}\left[h\left(X\right) F\left(X, X'\right)\right] < \infty$. Then, $\mathbb{E}\left[h\left(X\right) f\left(X\right)\right] = \mathbb{E}\left[h\left(X\right) F\left(X, X'\right)\right]$. Using the exchangeability of X and X' and the fact that F is antisymmetric, we have that

$$\mathbb{E}\left[h\left(X\right) F\left(X, X'\right)\right] = \mathbb{E}\left[h\left(X'\right) F\left(X', X\right)\right] = -\mathbb{E}\left[h\left(X'\right) F\left(X, X'\right)\right]$$

and that therefore

$$\mathbb{E}\left[h\left(X\right) f\left(X\right)\right] = \frac{1}{2}\mathbb{E}\left[\left(h\left(X\right) - h\left(X'\right)\right) F\left(X, X'\right)\right]. \tag{E.3}$$

Let

$$m(\theta) = \mathbb{E}\left[\exp\left(\theta f(X)\right)\right]$$

denote the moment generating function of $f(X)$. As $f(X)$ is bounded almost surely, we can exchange differentiation and expectation in the differentiation of $m(\theta)$. Thus, we obtain

$$\begin{aligned} m'(\theta) &= \mathbb{E}\left[\exp\left(\theta f(X)\right) f(X)\right]. \\ &= \frac{1}{2}\mathbb{E}\left[\left(\exp\left(\theta f(X)\right) - \exp\left(\theta f(X')\right)\right) F(X, X')\right], \end{aligned} \tag{E.4}$$

where the second inequality follows from (E.3). To bound $m'(\theta)$ we apply the following exponential mean-value inequality, stated in a more general form in Paulin et al. (2016).

Lemma E.2. *For all constants x, y, and c in $\mathbb{R}$ and $s > 0$, it holds that*

$$\left|\left(e^x - e^y\right) c\right| \leq \frac{1}{4}\left(s(x-y)^2 + s^{-1}c^2\right)\left(e^x + e^y\right).$$

In particular, by (E.4) and Lemma E.2, we obtain the bound

$$\begin{aligned} |m'(\theta)| &\leq \frac{1}{2}\mathbb{E}\left[\left|\left(\exp\left(\theta f(X)\right) - \exp\left(\theta f(X')\right)\right) F(X, X')\right|\right] \\ &\leq \frac{1}{8}\inf_{t>0}\mathbb{E}\left[\left(t\left(\theta f(X) - \theta f(X')\right)^2 + t^{-1}F(X, X')^2\right)\left(\exp\left(\theta f(X)\right) + \exp\left(\theta f(X')\right)\right)\right] \\ &= \frac{|\theta|}{4}\inf_{t>0}\mathbb{E}\left[\left(t\left(f(X) - f(X')\right)^2 + t^{-1}F(X, X')^2\right)\exp\left(\theta f(X)\right)\right] \\ &= \frac{|\theta|}{2}\inf_{t>0}\mathbb{E}\left[\left(\frac{t}{2}\mathbb{E}\left[\left(f(X) - f(X')\right)^2 \mid X\right] + \frac{1}{2t}\mathbb{E}\left[F(X, X')^2 \mid X\right]\right)\right. \\ &\qquad\qquad \left.\cdot\,\mathbb{E}\left[\exp\left(\theta f(X)\right) \mid X\right]\right] \\ &= \frac{|\theta|}{2}\inf_{t>0}\mathbb{E}\left[\left(tU_f(X) + t^{-1}U_F(X)\right)\mathbb{E}\left[\exp\left(\theta f(X)\right) \mid X\right]\right] \\ &\leq \frac{|\theta|}{2}\mathbb{E}\left[\left(sU_f(X) + s^{-1}U_F(X)\right)\mathbb{E}\left[\exp\left(\theta f(X)\right) \mid X\right]\right] \\ &\leq |\theta| v \mathbb{E}\left[\exp\left(\theta f(X)\right)\right] \end{aligned}$$

for all $\theta \in \mathbb{R}$. Thus, we have that

$$m'(\theta) \leq u\theta m(\theta)$$

for all $\theta > 0$. As $m(\cdot)$ is a convex function and $m'(0) = 0$, $m'(\theta)$ always has the same sign as θ, we find that

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\log m(\theta) \leq u\theta.$$

As a consequence, and by $m(0) = 1$, we have that

$$\log m(\theta) \leq \int_0^\theta ut\mathrm{d}t \leq \frac{u\theta^2}{2}.$$

By the Chernoff bound (see e.g., Equation 2.5, Wainwright, 2019), we have

$$\log P\{f(X) \geq \delta\} \leq \inf_{\theta \geq 0} (\log m(\theta) - \theta\delta) \leq \inf_{\theta \geq 0} \left(\frac{u\theta^2}{2} - \theta\delta\right)$$

Solving this minimization with $\theta = \delta/u$, we find

$$P\{f(X) \geq t\} \leq \exp\left(\frac{-\delta^2}{2u}\right),$$

as required. The analogous lower tail bound follows from an identical argument, which completes the proof of (D.26). To prove (D.27) we apply the following result stated in Chatterjee (2007).

Theorem E.1 (Theorem 1.5, (iii), Chatterjee, 2007)**.** *Reintroduce the notation and assumptions from the statement of Theorem D.2. Define*

$$\Delta(X) = \frac{1}{2}\mathbb{E}\left[|F(X, X')(f(X) - f(X'))| \mid X\right].$$

The Burkholder-Davis-Gundy inequality

$$\mathbb{E}\left[f(X)^{2r}\right] \leq (2r-1)^r \mathbb{E}\left[\Delta(X)^r\right]$$

holds for any positive integer r.

The inequality

$$\begin{aligned}
\mathbb{E}\left[\Delta(X)^r\right] &= \mathbb{E}\left[\mathbb{E}\left[|(f(X) - f(X'))F(X, X')| \mid X\right]^r\right] \\
&\leq \mathbb{E}\left[\mathbb{E}\left[|(f(X) - f(X'))F(X, X')|^r \mid X\right]\right] && \text{(Jensen)} \\
&= \mathbb{E}\left[\mathbb{E}\left[\left(\left(s^{-1}(f(X) - f(X'))^{2r}\right)\left(sF(X, X')^{2r}\right)\right)^{1/2} \mid X\right]\right] \\
&\leq \mathbb{E}\left[\mathbb{E}\left[s^{-1}(f(X) - f(X'))^{2r} + sF(X, X')^{2r} \mid X\right]\right] && \text{(Young)} \\
&= s^{-1}\mathbb{E}\left[U_f^{(r)}(X)\right] + s\mathbb{E}\left[U_F^{(r)}(X)\right]
\end{aligned}$$

then completes the proof. ■

E.3 Proof of Lemma D.3

We apply the following Lemma.

Lemma E.3. *Let $(X_m)_{m \geq 0}$ be a sequence of real-valued random variables. Suppose that the inequality*

$$\mathbb{E}\left[X_m^{2^c}\right] \leq h_m^{2^c} \tag{E.5}$$

holds for each $m \geq 0$ and positive integer c, where $(h_m)_{m\geq 0}$ is a deterministic sequence of nonnegative real numbers. If there exists a square integrable random variable W such that

$$\left(\sum_{m=0}^{\infty} X_m\right)^{2^c} \leq W$$

almost surely, then the inequality

$$\mathbb{E}\left[\left(\sum_{m=0}^{\infty} X_m\right)^{2^c}\right] \leq \left(\sum_{m=0}^{\infty} h_m\right)^{2^c}$$

holds almost surely.

Define the objects

$$U_f^{(r)}(Z) = \frac{1}{2}\mathbb{E}\left[\left(f(Z) - f(Z')\right)^{2r} \mid Z\right] \quad \text{and}$$

$$U_F^{(r)}(Z) = \frac{1}{2}\mathbb{E}\left[\left(\sum_{m=0}^{\infty} \mathbb{E}\left[f(Z_m) - f(Z'_m) \mid Z_0 = Z, Z'_0 = Z'\right]\right)^{2r} \mid Z\right].$$

By the (D.28), we have that

$$\mathbb{E}\left[\sum_{m=0}^{\infty} f(Z_m) - f(Z'_m) \mid Z_0 = Z, Z'_0 = Z'\right]^{2^c} \leq W.$$

Thus, (D.29) guarantees that the conditions of Lemma E.3 are satisfied, and we have that

$$\mathbb{E}\left[U_F^{(2^{c-1})}(Z) \mid \boldsymbol{\pi}\right] \leq \frac{1}{2}\left(\sum_{i=0}^{\infty} h_i\right)^{2^c} \quad \text{and} \quad \mathbb{E}\left[U_f^{(2^{c-1})}(Z) \mid \boldsymbol{\pi}\right] \leq \frac{1}{2}h_0^{2^c}.$$

By Markov's inequality, we obtain

$$P\left\{U_F^{(2^{c-1})}(Z) \geq \frac{2}{\delta}\mathbb{E}\left[U_F^{(2^{c-1})}(Z) \mid \boldsymbol{\pi}\right] \quad \text{or} \quad U_f^{(2^{c-1})}(Z) \geq \frac{2}{\delta}\mathbb{E}\left[U_f^{(2^{c-1})}(Z) \mid \boldsymbol{\pi}\right] \mid \boldsymbol{\pi}\right\} \leq \delta.$$

Hence, by Lemma E.3 and DeMorgan's law, the probability that both

$$U_F^{(2^{c-1})}(Z) \leq \frac{2}{\delta}\mathbb{E}\left[U_F^{(2^{c-1})}(Z) \mid \boldsymbol{\pi}\right] \leq \frac{1}{\delta}\left(\sum_{m=0}^{\infty} h_m\right)^{2^c} \quad \text{and}$$

$$U_f^{(2^{c-1})}(Z) \leq \frac{2}{\delta}\mathbb{E}\left[U_f^{(2^{c-1})}(Z) \mid \boldsymbol{\pi}\right] \leq \frac{h_0^{2^c}}{\delta}$$

hold is greater than $1 - \delta$. ■

E.4 Proof of Lemma D.4

Recall the definition of the collections $(\boldsymbol{\pi}_m, \boldsymbol{\pi}'_m)_{m\geq 0}$ given in (D.22). Fix $Z_0 = Z$ and $Z'_0 = Z'$ throughout. For any i in $[n]$, let $\mathsf{s}_{m,\ell}(i)$ denote the element of the collection

$$\mathsf{r}(\pi_{m,\ell}) = (\mathsf{s}_1(\pi_{m,\ell}), \ldots, \mathsf{s}_g(\pi_{m,\ell}))$$

that contains the index i and set $\mathsf{s}_{m,\ell}(i)$ equal to $\varnothing$ if no element of $\mathsf{r}(\pi_{m,\ell})$ contains i.

We begin by defining three events that will determine the structure of our argument. By construction, the collections $\boldsymbol{\pi}_m$ and $\boldsymbol{\pi}'_m$ are either identical or differ in exactly two indices in their Lth element. Let $\mathcal{E}_m$ denote the event that $\boldsymbol{\pi}_m$ and $\boldsymbol{\pi}'_m$ differ. On the event $\mathcal{E}_m$, let $i_{1,m}$ and $i_{2,m}$ denote the two indices in which the Lth elements of $\boldsymbol{\pi}_m$ and $\boldsymbol{\pi}'_m$ differ. Define the random variables B_m and C_m such that, conditional on $\mathcal{E}_m$, each is uniformly distributed on $\{i_{1,m}, i_{2,m}\}$ such that $B_m \neq C_m$. On the complement of $\mathcal{E}_m$, set these indices uniformly at random. Let $\mathcal{F}_m$ denote the event that

$$\mathsf{s}_{m,L}(B_m) \neq \mathsf{s}_{m,L}(C_m),$$

i.e., the event that the indices that differ are not in the same element of the collection $\mathsf{r}(\pi_{m,\ell})$. Finally, let $\mathcal{G}_m$ denote the event that

$$\mathsf{s}_{m,L}(B_m) \neq \varnothing \quad \text{and} \quad \mathsf{s}_{m,L}(C_m) \neq \varnothing,$$

i.e., the event that the indices that differ are both in the collection $\mathsf{r}(\pi_{m,\ell})$.

By Assumption 4.1, the event $\mathcal{H}_m = \mathcal{E}_m \cap \mathcal{F}_m$ is a necessary condition for $a(Z_m) - a(Z'_m) \neq 0$. Thus, we can compute

$$\begin{aligned}
P\{\mathcal{H}_m \mid \mathcal{E}_0\} &= P\{\mathcal{F}_m \mid \mathcal{E}_m, \mathcal{E}_0\} P\{\mathcal{E}_m \mid \mathcal{E}_0\} \\
&= \Big(P\{\mathsf{s}_{m,L}(B_m) \neq \mathsf{s}_{m,L}(C_m) \mid \mathsf{s}_{m,L}(B_m) \neq \varnothing, \mathcal{E}_m\} P\{\mathsf{s}_{m,L}(B_m) \neq \varnothing \mid \mathcal{E}_m\} \\
&\quad + P\{\mathsf{s}_{m,L}(B_m) \neq \mathsf{s}_{m,L}(C_m) \mid \mathsf{s}_{m,L}(B_m) = \varnothing, \mathcal{E}_m\} P\{\mathsf{s}_{m,L}(B_m) = \varnothing \mid \mathcal{E}_m\} \Big) \\
&\quad \cdot P\{\mathcal{E}_m \mid \mathcal{E}_0\} \\
&= \left(\frac{n-b}{n-1}\frac{kb}{n} + \frac{kb}{n-1}\frac{n-kb}{b} \right) \left(1 - \frac{2}{gn^2}\right)^m \\
&= \left(\frac{kb(2n-kb-b)}{n(n-1)} \right) \left(1 - \frac{2}{gn^2}\right)^m
\end{aligned}$$

for all $m \geq 0$ by the law of total probability. Moreover, we have that

$$P\{\mathcal{H}_m \mid Z, Z'\} \leq P\{\mathcal{H}_m \mid \mathcal{E}_0\}$$

almost surely. Consequently, we find that

$$\begin{aligned}
&\mathbb{E}\left[\mathbb{E}\left[a\left(Z_m\right)-a\left(Z_m'\right) \mid Z, Z'\right]^{2r} \mid \boldsymbol{\pi}\right] \\
&=\mathbb{E}\left[\left(P\left\{\mathcal{H}_m \mid Z, Z'\right\} \mathbb{E}\left[a\left(Z_m\right)-a\left(Z_m'\right) \mid Z, Z', \mathcal{H}_m\right]\right)^{2r} \mid \boldsymbol{\pi}\right] \\
&\leq\left(P\left\{\mathcal{H}_m \mid \mathcal{E}_0\right\}\right)^{2r} \mathbb{E}\left[\mathbb{E}\left[\left(a\left(Z_m\right)-a\left(Z_m'\right)\right)^{2r} \mid Z, Z', \mathcal{H}_m\right] \mid \boldsymbol{\pi}\right] \qquad \text{(Jensen)} \\
&=\left(1-\frac{2}{gn^2}\right)^{2mr}\left(\frac{kb\left(2n-kb-b\right)}{n(n-1)}\right)^{2r} \mathbb{E}\left[\mathbb{E}\left[\left(a\left(Z_m\right)-a\left(Z_m'\right)\right)^{2r} \mid \mathcal{H}_m, \boldsymbol{\pi}\right] \mid \boldsymbol{\pi}\right] \\
&\leq\left(1-\frac{2}{gn^2}\right)^{2mr}\left(\frac{2kb\left(2n-kb-b\right)}{n^2}\right)^{2r} \mathbb{E}\left[\left(a\left(Z_m\right)-a\left(Z_m'\right)\right)^{2r} \mid \mathcal{H}_m\right], \qquad \text{(E.6)}
\end{aligned}$$

where the final inequality follows from the fact that $\boldsymbol{\pi}$ is uniformly distributed independently of D and the elementary inequality $n/(n-1) \leq 2$. Thus, it remains to bound the expectation in (E.6).

To ease notation, we now drop the dependence on m and L. Observe that

$$P\left\{\mathcal{G} \mid \mathcal{H}\right\}=P\left\{\mathsf{s}\left(B\right) \neq \varnothing \mid \mathsf{s}\left(C\right) \neq \varnothing\right\}=\frac{kb-b}{n-b}$$

and that therefore

$$\begin{aligned}
\mathbb{E}\left[\left(a\left(Z\right)-a\left(Z'\right)\right)^{2r} \mid \mathcal{H}, \boldsymbol{\pi}\right] &= \left(\frac{kb-b}{n-b}\right) \mathbb{E}\left[\left(a\left(Z\right)-a\left(Z'\right)\right)^{2r} \mid \mathcal{G}\right] \\
&\quad+\left(\frac{n-kb}{n-b}\right) \mathbb{E}\left[\left(a\left(Z\right)-a\left(Z'\right)\right)^{2r} \mid \mathcal{H} \setminus \mathcal{G}\right]. \qquad \text{(E.7)}
\end{aligned}$$

Define the sets

$$\hat{\mathsf{s}}_i=\mathsf{s}(i) \setminus i \quad \text{and} \quad \bar{\mathsf{s}}=\tilde{\mathsf{s}}(B) \cap \tilde{\mathsf{s}}(C).$$

With an abuse of notation, we let

$$\begin{aligned}
\psi(D_i, \hat{\eta}(D_j, D_{\hat{\mathsf{s}}_k}))=\psi(D_i, \hat{\eta}(D_j \cap D_{\hat{\mathsf{s}}_k} \cap D_{\bar{\mathsf{s}}})) \quad \text{and} \\
h(D_i, D_j, D_{\hat{\mathsf{s}}_k})=\psi(D_i, \hat{\eta}(D_j, D_{\hat{\mathsf{s}}_k}))-\psi(D_j, \hat{\eta}(D_i, D_{\hat{\mathsf{s}}_k})).
\end{aligned}$$

Observe that

$$\begin{aligned}
&\mathbb{E}\left[\left(a\left(Z\right)-a\left(Z'\right)\right)^{2r} \mid \mathcal{H} \setminus \mathcal{G}\right] \\
&=\mathbb{E}\left[\left(a\left(Z\right)-a\left(Z'\right)\right)^{2r} \mid \mathcal{H} \setminus \mathcal{G}\right]=\left(\frac{1}{gkb}\right)^{2r} \mathbb{E}\left[h(D_B, D_C, D_{\tilde{s}_C})^{2r}\right]. \qquad \text{(E.8)}
\end{aligned}$$

On the other hand, we can decompose

$$\begin{aligned}
&\mathbb{E}\left[\left(a\left(Z\right)-a\left(Z'\right)\right)^{2} \mid \mathcal{G}\right] \\
&=\left(\frac{1}{gkb}\right)^{2r} \mathbb{E}\left[\left(h(D_B, D_C, D_{\hat{\mathsf{s}}_C})+h(D_C, D_B, D_{\hat{\mathsf{s}}_B})\right)^{2r}\right]
\end{aligned}$$

$$= \left(\frac{1}{gkb}\right)^{2r} \mathbb{E}\left[\left(h(D_B, D_C, D_{\hat{\mathsf{s}}_C}) - h(D_B, D_B, D_{\hat{\mathsf{s}}_B})\right)^{2r}\right] . \tag{E.9}$$

Consequently, by (E.7), (E.8), and (E.9), it suffices to express suitable bounds for the expectations

$$\begin{aligned} &\mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C}))\right)^{2r}\right] \quad \text{and} \\ &\mathbb{E}\Bigg[\Bigg(\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C}))\right) \\ &\qquad - \left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_B})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_B}))\right) \Bigg)^{2r}\Bigg] \end{aligned} \tag{E.10}$$

respectively. To this end, recall that $\tilde{D}_i$ are independent copies of D_i for each i. Observe that

$$\begin{aligned} &\mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C}))\right)^{2r}\right] \\ &= \mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C})) + \psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C}))\right)^{2r}\right] \\ &= \sum_{q=0}^{2r} \binom{2r}{q} \mathbb{E}\Bigg[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C}))\right)^{2r-q} \\ &\qquad \left(\psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C}))\right)^{q} \Bigg] \qquad \text{(Binomial Theorem)} \\ &\leq 2^{2r} \mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C}))\right)^{2r}\right] \end{aligned} \tag{E.11}$$

where the inequality follows from the fact that B and C are exchangeable and the Hölder inequality. Similarly, we have that

$$\begin{aligned} &\mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C}))\right)^{2r-q}\right] \\ &= \mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C})) + \psi(D_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C})) - \psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C}))\right)^{2r}\right] \\ &= \sum_{q=0}^{2r} \binom{2r}{q} \mathbb{E}\Bigg[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C}))\right)^{2r-q} \\ &\qquad \left(\psi(D_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C})) - \psi(\tilde{D}_B, \hat{\eta}(\tilde{D}_C, D_{\hat{\mathsf{s}}_C}))\right)^{q} \Bigg] \qquad \text{(Binomial Theorem)} \\ &\leq \sum_{q=0}^{2r} \binom{2r}{q} \left(\sigma_{\mathsf{valid}}^{(2r)}\right)^{\frac{2r-q}{2r}} \left(\sigma_{\mathsf{train}}^{(2r,1)}\right)^{\frac{q}{2r}} \qquad \text{(Hölder)} \\ &\leq 2^{2r} \sigma_{\mathsf{max}}^{(2r)}, \end{aligned} \tag{E.12}$$

where the last inequality follows by the definitions of $\sigma^{(2r)}_{\mathsf{valid}}$ and $\sigma^{(2r,1)}_{\mathsf{train}}$. Thus, we have that

$$\mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C}))\right)^{2r}\right] \leq 2^{4r}\sigma^{(2r)}_{\mathsf{max}} \tag{E.13}$$

by (E.11) and (E.12).

Next, we consider the double difference term (E.10). In this case, we have that

$$\begin{aligned}
&\mathbb{E}\Bigg[\Bigg((\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C}))) \\
&\qquad - (\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_B})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_B}))) \Bigg)^{2r}\Bigg] \\
&= \mathbb{E}\Bigg[\Bigg((\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_B}))) \\
&\qquad - (\psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_B}))) \Bigg)^{2r}\Bigg] \\
&= \sum_{q=0}^{2r} \binom{2r}{q} \mathbb{E}\Bigg[\Bigg((\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_B}))) \\
&\qquad \cdot (\psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_C})) - \psi(D_C, \hat{\eta}(D_B, D_{\hat{\mathsf{s}}_B}))) \Bigg)^{2r}\Bigg] \qquad \text{(Binomial Theorem)} \\
&\leq 2^{2r}\mathbb{E}\left[\left(\psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_C})) - \psi(D_B, \hat{\eta}(D_C, D_{\hat{\mathsf{s}}_B}))\right)^{2r}\right] = 2^{2r}\sigma^{(2r,b-1)}_{\mathsf{train}}
\end{aligned} \tag{E.14}$$

where the final inequality follows from the fact that B and C are exchangeable and the Hölder inequality. Putting the pieces together, we have that

$$\begin{aligned}
&\mathbb{E}\left[\mathbb{E}\left[a\left(Z_m\right) - a\left(Z'_m\right) \mid Z, Z'\right]^{2r} \mid \boldsymbol{\pi}\right] \\
&\leq 2^{4r}\left(1 - \frac{2}{gn^2}\right)^{2mr}\left(\frac{2n - kb - b}{gn^2}\right)^{2r}\left(\left(\frac{n - kb}{n - b}\right)2^{2r}\sigma^{(2r)}_{\mathsf{max}} + \left(\frac{kb - b}{n - b}\right)\sigma^{(2r,b-1)}_{\mathsf{train}}\right)
\end{aligned}$$

as required. ■

E.5 Proof of Lemma D.5

Throughout, we us the short hand $\hat{v}_{g,k}\left(Z\right)$ to denote $\hat{v}(\mathsf{R}_{g,k}, D)$. We begin by decomposing the estimator $\hat{v}_{g,k}\left(Z\right)$ into two parts that will each be easier to handle when considered in isolation. To this end, define the statistics

$$\begin{aligned}
\tilde{v}_{g,k}\left(Z\right) &= \frac{1}{g^2k^2}\sum_{\ell=1}^{g}\sum_{i,i'=1}^{k}\left(T(\mathsf{s}_{\ell,i}, Y) - \overline{a}\left(D\right)\right)\left(T(\mathsf{s}_{\ell,i'}, D) - \overline{a}\left(D\right)\right) \quad \text{and} \\
\check{v}_{g,k}\left(Z\right) &= \left(a\left(Z\right) - \overline{a}\left(D\right)\right)^2.
\end{aligned}$$

Observe that both $\tilde{v}_{g,k}(Z)$ and $\check{v}_{g,k}(Z)$ are unbiased for $v(Z)$. Moreover, we can write

$$\begin{aligned}
\hat{v}_{g,k}(Z) &= \frac{1}{g(g-1)k^2}\sum_{\ell=1}^{g}\sum_{i,i'=1}^{k}\left(T(\mathsf{s}_{\ell,i},D)-a(Z)\right)\left(T(\mathsf{s}_{\ell,i'},D)-a(Z)\right) \\
&= \frac{1}{g(g-1)k^2}\sum_{\ell=1}^{g}\sum_{i,i'=1}^{k}\left(T(\mathsf{s}_{\ell,i},D)-\overline{a}(D)\right)\left(T(\mathsf{s}_{\ell,i'},D)-a(Z)\right) \\
&\quad + \frac{1}{g(g-1)k}\sum_{\ell=1}^{g}\sum_{i=1}^{g}\left(\overline{a}(D)-a(Z)\right)\left(T(\mathsf{s}_{\ell,i},D)-a(Z)\right) \\
&= \frac{1}{g(g-1)k^2}\sum_{\ell=1}^{g}\sum_{i,i'=1}^{k}\left(T(\mathsf{s}_{\ell,i},D)-\overline{a}(D)\right)\left(T(\mathsf{s}_{\ell,i'},D)-a(Z)\right) \\
&= \frac{g}{g-1}\tilde{v}(Z)+\frac{1}{g(g-1)k}\sum_{\ell=1}^{g}\sum_{i=1}^{k}\left(T(\mathsf{s}_{\ell,i},D)-\overline{a}(D)\right)\left(\overline{a}(D)-a(Z)\right) \\
&= \frac{g}{g-1}\tilde{v}_{g,k}(Z)-\frac{1}{g-1}\check{v}_{g,k}(Z). \qquad \text{(E.15)}
\end{aligned}$$

Hence, it will suffice to characterize the exponential rates of conditional concentration for the statistics $\tilde{v}_{g,k}(Z)$ and $\check{v}_{g,k}(Z)$. These are established through the application of the following Lemma, which follows from an argument very similar to the proof of Theorem D.1.

Lemma E.4. *Suppose that Assumptions 4.1 and 4.2 hold and that the data D are independently and identically distributed. If the eighth-order split-stability $\zeta^{(8)}$ is finite, then:*
(i) *The conditional concentration inequality*

$$\log\frac{1}{2}P\left\{|\tilde{v}(Z)-v(D)|\geq t\mid D\right\}\lesssim -\frac{\delta}{(2-\varphi k-\varphi)^4}\frac{g^3t^2}{\Gamma^{(2)}_{k,\varphi,b}}, \qquad \text{(E.16)}$$

holds for all $t>0$ with probability greater than $1-\delta$.
(ii) *The conditional concentration inequality*

$$\log\frac{1}{2}P\left\{|\check{v}(Z)-v(D)|\geq t\mid D\right\}\lesssim -\frac{\delta}{(2-\varphi k-\varphi)^4}\frac{g^2t^2}{\Gamma^{(2)}_{k,\varphi,b}}, \qquad \text{(E.17)}$$

holds for all $t>0$ with probability greater than $1-\delta$.

Putting the pieces together, by (E.15), we have that

$$\begin{aligned}
&P\left\{|\hat{v}_{g,k}(Z)-v_{g,k}(D)|\leq t\mid D\right\} \\
&= P\left\{|\frac{g}{g-1}\left(\tilde{v}_{g,k}(Z)-v_{g,k}(D)\right)-\frac{1}{g-1}\left(\check{v}_{g,k}(Z)-v_{g,k}(D)\right)|\leq t\mid D\right\} \\
&\geq P\left\{\frac{g}{g-1}|\tilde{v}_{g,k}(Z)-v_{g,k}(D)|+\frac{1}{g-1}|\check{v}_{g,k}(Z)-v_{g,k}(D)|\leq t\mid D\right\}
\end{aligned}$$

$$\geq P\left\{\frac{g}{g-1}|\tilde{v}_{g,k}\left(Z\right)-v\left(D\right)|\leq\frac{\sqrt{g}}{1+\sqrt{g}}t,\frac{1}{g-1}|\check{v}\left(Z\right)-v\left(D\right)|\leq\frac{1}{1+\sqrt{g}}t\mid D\right\}$$
$$\geq P\left\{|\tilde{v}_{g,k}\left(Z\right)-v\left(D\right)|\leq\frac{1}{\sqrt{g}}\frac{g-1}{1+\sqrt{g}}t\mid D\right\}+P\left\{|\check{v}_{g,k}\left(Z\right)-v\left(D\right)|\leq\frac{g-1}{1+\sqrt{g}}t\mid D\right\}-1$$
$$\geq 1-4\exp\left(-\frac{\delta}{C(2-\varphi k-\varphi)^{4}}\frac{g^{3}t^{2}}{\Gamma_{k,\varphi,b}^{(2)}}\right)$$

with probability greater than $1-\delta$ for some universal constant C, where the last inequality follows by Lemma E.4 and the facts that $4g\geq\left(1+\sqrt{g}\right)^{2}$ for all $g\geq 1$ and $\left(1/4\right)g^{2}\leq\left(g-1\right)^{2}$ for all $g\geq 2$. ■

E.6 Proof of Lemma D.6

Define the event

$$\mathcal{W}_{\lambda}\left(D\right)=\mathcal{U}_{k,\lambda}\left(D\right)\cap\mathcal{Q}_{k,\lambda}(D),$$

the quantity

$$W\left(D\right)=\left(U(\mathsf{R}_{\hat{g},k},D)-U(\mathsf{R}'_{\hat{g}',k},D\right)+\left(Q(\mathsf{R}_{\hat{g},k},D)-Q(\mathsf{R}'_{\hat{g}',k},D)\right).$$

By the decomposition (C.6), we have that

$$\left|P\left\{a(\mathsf{R}_{\hat{g},k},D)-a(\mathsf{R}'_{\hat{g}',k},D)\leq\xi\mid D\right\}-(1-\beta/2)\right|$$
$$=\left|P\left\{\frac{a(\mathsf{R}_{\hat{g},k},D)-a(\mathsf{R}'_{\hat{g}',k},D)}{\sqrt{2v_{g^{\star},k}\left(D\right)}}\leq\frac{\xi}{\sqrt{2v_{g^{\star},k}\left(D\right)}}\mid D\right\}-(1-\beta/2)\right|$$
$$=\left|P\left\{\frac{a(\mathsf{R}_{g^{\star},k},D)-a(\mathsf{R}'_{g^{\star},k},D)}{\sqrt{2v_{g^{\star},k}\left(D\right)}}\leq\frac{\xi}{\sqrt{2v_{g^{\star},k}\left(D\right)}}-\frac{W\left(D\right)}{\sqrt{2v_{g^{\star},k}\left(D\right)}}\mid D\right\}-(1-\beta/2)\right|$$
$$\leq\sup_{q\in[-2\lambda,2\lambda]}\left|P\left\{\frac{a(\mathsf{R}_{g^{\star},k},D)-a(\mathsf{R}'_{g^{\star},k},D)}{\sqrt{2v_{g^{\star},k}\left(D\right)}}\leq z_{1-\beta/2}+q\right\}-(1-\beta/2)\right|$$
$$+\left(1-P\left\{\mathcal{W}_{\lambda}\left(D\right)\mid D\right\}\right)$$
$$\leq\sup_{z\in\mathbb{R}}\left|P\left\{\frac{a(\mathsf{R}_{g^{\star},k},D)-a(\mathsf{R}'_{g^{\star},k},D)}{\sqrt{2v_{g^{\star},k}\left(D\right)}}\leq z\mid D\right\}-\Phi(z)\right|+2\lambda+\left(1-P\left\{\mathcal{W}_{\lambda}\left(D\right)\mid D\right\}\right),$$

as required. ■

E.7 Proof of Lemma D.7

E.7.1 Part (i). Observe that we can write

$$a(\mathsf{R}_{g^{\star},k},D)-a(\mathsf{R}'_{g^{\star},k},D)=\frac{1}{g^{\star}}\sum_{\ell=1}^{g}\left(\overline{a}(\mathsf{r}_{\ell},D)-\overline{a}(\mathsf{r}'_{\ell},D)\right),$$

where $\overline{a}(\cdot, D)$ is defined in (D.33). We have that

$$\begin{aligned}\mathbb{E}\left[|\overline{a}(\mathsf{r}_\ell, D) - \overline{a}(\mathsf{r}'_\ell, D)|^3\right] &\leq \left(\mathbb{E}\left[(\overline{a}(\mathsf{r}_\ell, D) - \overline{a}(\mathsf{r}'_\ell, D))^4\right]\right)^{3/4} \qquad \text{(Hölder)}\\ &\leq 2^6\left(\mathbb{E}\left[(\overline{a}(\mathsf{r}_\ell, D))^4\right]\right)^{3/4}\\ &\leq 2^6 3^2 (2-\varphi k-\varphi)^3 (\Gamma^{(2)}_{k,\varphi,b})^{3/4}\,,\end{aligned}$$

where the second inequality follows from Hölder's inequality, the binomial theorem, and the fact that r_ℓ and r'_ℓ are exchangeable. The final inequality follows from Theorem D.2. Consequently, we find that

$$\begin{aligned}\frac{\mathbb{E}\left[|\overline{a}(\mathsf{r}_\ell, D) - \overline{a}(\mathsf{r}'_\ell, D)|^3 \mid D\right]}{(g^\star)^{1/2}\left(2v_{1,k}(D)\right)^{3/2}} &\lesssim \frac{(2-\varphi k-\varphi)^3(\Gamma^{(2)}_{k,\varphi,b})^{3/4}}{\delta\,(g^\star)^{1/2}\left(v_{1,k}(D)\right)^{3/2}} \qquad \text{(Markov)}\\ &\lesssim \frac{\xi}{z_{1-\beta/2}}\frac{(2-\varphi k-\varphi)^3(\Gamma^{(2)}_{k,\varphi,b})^{3/4}}{\delta\left(v_{1,k}(D)\right)^2}\,,\end{aligned}$$

holds with probability $1-\delta$. The Lemma then follows by the Berry-Esseen inequality. ■

E.7.2 Part (ii). Our bound is based on the following two conditional concentration inequalities. Both arguments are based on a Chernoff-type maximal inequality, due to Steiger (1970).

Lemma E.5. *Suppose that Assumptions 4.1 and 4.2 hold, that the data D are independent and identically distributed, and that the eighth-order split ζ^8 stability is finite.*
(i) *For all $t>0$ and $c>0$, the condition concentration inequality*

$$\log\frac{1}{2}P\left\{|U(\mathsf{R}_{\hat{g},k}, D)| \geq t\sqrt{v_{g^\star,k}(D)}, |\hat{g}/g^\star - 1| \leq c \mid D\right\} \tag{E.18}$$

$$\leq -\frac{\delta v_{1,k}(D)}{2^4(2-\varphi k-\varphi)^2\Gamma^{(1)}_{k,\varphi,b}}\frac{t^2}{c} \tag{E.19}$$

holds with probability greater than $1-\delta$ as D varies.
(ii) *If $g^\star c \geq 2$ and $1/2 > c > 0$, then the conditional concentration inequality*

$$\log\frac{1}{8}P\left\{|\hat{g}-g^\star| > cg^\star \mid D\right\} \lesssim -\frac{\delta(v_{1,k}(D))^3}{(2-\varphi k-\varphi)^4}\frac{z^2_{1-\beta/2}}{\Gamma^{(2)}_{k,\varphi,b}}\frac{c^2}{\xi^2} \tag{E.20}$$

holds with probability greater than $1-\delta$ as D varies.

Observe that

$$\begin{aligned}&P\left\{|U(\mathsf{R}_{\hat{g},k}, D) - U(\mathsf{R}'_{\hat{g}',k}, D)| \geq \lambda\sqrt{2v_{g^\star,k}(D)}\right\}\\ &\lesssim P\left\{|U(\mathsf{R}_{\hat{g},k}, D)| \geq \lambda\sqrt{2v_{g^\star,k}(D)}\right\}\end{aligned}$$

$$\leq P\left\{|U(\mathsf{R}_{\hat{g},k},D)|\geq\lambda\sqrt{2v_{g^\star,k}\left(D\right)},|\hat{g}/g^\star-1|\leq c\mid D\right\}+P\left\{|\hat{g}/g^\star-1|\geq c\mid D\right\}$$

$$\lesssim\exp\left(-\frac{\delta v_{1,k(D)}}{2^4(2-\varphi k-\varphi)^2\Gamma^{(1)}_{k,\varphi,b}}\frac{\lambda^2}{c}\right)+\exp\left(-C\frac{\delta(v_{1,k}(D))^3}{(2-\varphi k-\varphi)^4}\frac{z^2_{1-\beta/2}}{\Gamma^{(2)}_{k,\varphi,b}}\frac{c^2}{\xi^2}\right)\tag{E.21}$$

for some universal constant C. Hence, it remains to choose c and λ such that the quantity (E.21) is less than $\rho_{k,\varphi,b}\left(\xi,\beta\mid D\right)$. First, we choose c such that

$$\frac{\delta(v_{1,k}(D))^3}{(2-\varphi k-\varphi)^4}\frac{z^2_{1-\beta/2}}{\Gamma^{(2)}_{k,\varphi,b}}\frac{c^2}{\xi^2}\lesssim\log\left(\rho_{k,\varphi,b}\left(\xi,\beta\mid D\right)^{-1}\right)$$

Choosing c by

$$c=\xi\left(\frac{(2-\varphi k-\varphi)^2\left(\Gamma^{(2)}_{k,\varphi,b}\right)^{1/2}}{z_{1-\beta/2}\delta^{1/2}(v_{1,k}(D))^{3/2}}\right)\log^{1/2}\left(\rho_{k,\varphi,b}\left(\xi,\beta\mid D\right)^{-1}\right)\tag{E.22}$$

suffices. Next, we choose λ such that

$$\frac{\delta v_{1,k(D)}}{2^4(2-\varphi k-\varphi)^2\Gamma^{(1)}_{k,\varphi,b}}\frac{\lambda^2}{c}\lesssim\log\left(\rho_{k,\varphi,b}\left(\xi,\beta\mid D\right)^{-1}\right).$$

We can rewrite this condition by plugging in our choice of c through

$$\frac{\lambda^2}{\xi}\frac{z_{1-\beta/2}\delta^{3/2}(v_{1,k}(D))^{5/2}}{(2-\varphi k-\varphi)^4\Gamma^{(1)}_{k,\varphi,b}(\Gamma^{(2)}_{k,\varphi,b})^{1/2}}\lesssim\log^{3/2}\left(\rho_{k,\varphi,b}\left(\xi,\beta\mid D\right)^{-1}\right)$$

Choosing λ by

$$\lambda=\left(\frac{\xi}{z_{1-\beta/2}}\frac{(2-\varphi k-\varphi)^4\Gamma^{(1)}_{k,\varphi,b}(\Gamma^{(2)}_{k,\varphi,b})^{1/2}}{\delta^{3/2}(v_{1,k}\left(D\right))^{5/2}}\right)^{1/2}\tilde{\lambda}_{k,\varphi,b}\left(D\right),\quad\text{where}$$

$$\tilde{\lambda}_{k,\varphi,b}\left(D\right)=\log^{3/4}\left(\rho_{k,\varphi,b}\left(\xi,\beta\mid D\right)^{-1}\right)$$

will then suffice, as required. ■

E.7.3 Part(iii). Observe that

$$P\left\{|\left(1-\frac{\hat{g}}{g^\star}\right)\left(a(\mathsf{R}_{\hat{g},k},D)-\overline{a}\left(D\right)\right)|\geq\lambda\sqrt{2v_{g^\star,k}\left(D\right)},|g^\star-\hat{g}|\leq cg^\star\mid D\right\}$$

$$=P\left\{|\left(a(\mathsf{R}_{\hat{g},k},D)-\overline{a}\left(D\right)\right)|\geq\frac{\lambda}{c}\sqrt{2v_{g^\star,k}\left(D\right)},|g^\star-\hat{g}|\leq cg^\star\mid D\right\}$$

$$\leq P\left\{\max_{|g^\star-g|\leq cg^\star}|\left(a(\mathsf{R}_{g,k},D)-\overline{a}\left(D\right)\right)|\geq\frac{\lambda}{c}\sqrt{2v_{g^\star,k}\left(D\right)}\mid D\right\}$$

$$\leq P\left\{\max_{|g^\star-g|\leq cg^\star}|\left(a(\mathsf{R}_{g,k},D)-\overline{a}\left(D\right)\right)|\geq\frac{\lambda}{c}\left(\frac{\xi}{z_{1-\beta/2}}\right)\mid D\right\}$$

$$\leq \sum_{|g^\star - g| \leq cg^\star} P\left\{ \left| \left(a(\mathsf{R}_{g,k}, D) - \overline{a}\left(D\right) \right) \right| \geq \frac{\lambda}{c} \left(\frac{\xi}{z_{1-\beta/2}} \right) \right\} . \tag{E.23}$$

By Theorem D.1, we have that

$$\begin{aligned} & P\left\{ \left| \left(a(\mathsf{R}_{g,k}, D) - \overline{a}\left(D\right) \right) \right| \geq \frac{\lambda}{c} \left(\frac{\xi}{z_{1-\beta/2}} \right) \right\} \\ & \leq 2 \exp\left(- \frac{g\delta}{2^4 (2 - \varphi k - \varphi)^2 \Gamma_{k,\varphi,b}(1)} \frac{\lambda^2}{c^2} \left(\frac{\xi}{z_{1-\beta/2}} \right)^2 \right) \end{aligned}$$

and so is (E.23) bounded from above by

$$\begin{aligned} & 4cg^\star \exp\left(- \frac{g^\star (1-c)\delta}{4(2 - \varphi k - \varphi)^2 \Gamma_{k,\varphi,b}(1)} \frac{\lambda^2}{c^2} \left(\frac{\xi}{z_{1-\beta/2}} \right)^2 \right) \\ & \lesssim v_{1,k}\left(D\right) c \left(\frac{z_{1-\beta/2}}{\xi} \right)^2 \exp\left(- \frac{\delta v_{1,k}(D)}{2^5 (2 - \varphi k - \varphi)^2 \Gamma_{k,\varphi,b}(1)} \frac{\lambda^2}{c^2} \right) \end{aligned}$$

if $1 - c \geq 1/2$ by the definition of $g^\star$. Thus, we have that

$$\begin{aligned} & P\left\{ |Q(\mathsf{R}_{\hat{g},k}, D) - Q(\mathsf{R}'_{\hat{g}',k}, D)| \geq \lambda \sqrt{2 v_{g^\star,k}\left(D\right)} \mid D \right\} \\ & \lesssim P\left\{ \left| \left(1 - \frac{\hat{g}}{g^\star} \right) \left(a(\mathsf{R}_{\hat{g},k}, D) - \overline{a}\left(D\right) \right) \right| \geq \lambda \sqrt{2 v_{g^\star,k}\left(D\right)}, |g^\star - \hat{g}| \leq cg^\star \mid D \right\} \\ & + P\left\{ |g^\star - \hat{g}| \geq cg^\star \mid D \right\} \\ & \lesssim v_{1,k}\left(D\right) c \left(\frac{z_{1-\beta/2}}{\xi} \right)^2 \exp\left(- \frac{\delta v_{1,k}(D)}{2^5 (2 - \varphi k - \varphi)^2 \Gamma^{(1)}_{k,\varphi,b}} \frac{\lambda^2}{c^2} \right) \qquad \text{(E.24)} \\ & \quad + \exp\left(- \frac{1}{C} \frac{\delta (v_{1,k}(D))^3}{(2 - \varphi k - \varphi)^4} \frac{z_{1-\beta/2}}{\Gamma^{(2)}_{k,\varphi,b}} \frac{c^2}{\xi^2} \right) \qquad \text{(E.25)} \end{aligned}$$

for some universal constant C by Lemma E.5, Part (ii). If c is chosen to satisfy (E.22), the term (E.25) will be bounded above by $\rho_{\varphi,k}\left(\xi, \beta \mid D\right)$ for all sufficiently small ξ. By plugging this value of c and $\lambda = \lambda_{\varphi,k}\left(\xi, \beta \mid D\right)$ into (E.24), we obtain the term

$$\begin{aligned} & \left(\frac{z^2_{1-\beta/2}}{\xi} \right) \left(\frac{(2 - \varphi k - \varphi)^2 \left(\Gamma^{(2)}_{k,\varphi,b}\right)^{1/2}}{z_{1-\beta/2} \delta^{1/2} (v_{1,k}(D))^{1/2}} \right) \log^{1/2}\left(\rho_{k,\varphi,b}\left(\xi, \beta \mid D\right)^{-1} \right) \\ & \exp\left(- \frac{1}{\xi} \frac{\delta^{1/2} (v_{1,k}(D))^{3/2}}{(2 - \varphi k - \varphi)^2 (\Gamma^{(2)}_{k,\varphi,b})^{1/2}} \tilde{\lambda}^U_{k,\varphi,b}\left(D\right) \log\left(\rho_{k,\varphi,b}\left(\xi, \beta \mid D\right)^{-1} \right) \right) \qquad \text{(E.26)} \end{aligned}$$

as required. Observe that the term (E.26) is bounded above by $\rho_{\varphi,k}\left(\xi, \beta \mid D\right)$, for all sufficiently small ξ, completing the proof. ■

E.8 Proofs for Supporting Lemmas

E.8.1 Proof of Lemma E.1. Let $T_i(\pi_{m,\ell}) = T(\mathsf{s}_i(\pi_{\ell,m}), D)$ and define $T_i(\pi'_{m,\ell})$ analogously. Define

$$R_m(\ell) = \left\{ i \in [n] : \pi_{m,\ell}(i) \neq \pi'_{m,\ell}(i) \right\}$$

and let $\overline{R}_m(\ell) = |R_m(\ell)|$ denote the number of shared indices in the permutations in $\pi_{m,\ell}$ and $\pi'_{m,\ell}$. Observe that

$$\frac{1}{k}\sum_{i=1}^{k}\left(T_i(\pi_{m,\ell}) - T_i\left(\pi'_{m,\ell}\right)\right) = 0 \tag{E.27}$$

almost surely for all $m' \geq m$ if and only if $\overline{R}_m(\ell) = n$. Let $N(\ell)$ denote the values of the smallest index m with $\overline{R}_m(\ell) = n$. Observe that

$$\begin{aligned}
&\sum_{m=0}^{\infty}\left|\mathbb{E}\left[a(\mathsf{R}_{g,k}(\boldsymbol{\pi}_m), D) - a(\mathsf{R}_{g,k}(\boldsymbol{\pi}'_m), D) \mid \boldsymbol{\pi}_0 = \boldsymbol{\psi}, \boldsymbol{\pi}'_0 = \boldsymbol{\psi}', D\right]\right| \qquad \text{(E.28)}\\
&\leq \sum_{m=0}^{\infty}\frac{1}{g}\frac{1}{k}\sum_{\ell=1}^{g}\sum_{i=1}^{k}\mathbb{E}\left[\left|\left(T_i(\pi_{m,\ell}) - T_i\left(\pi'_{m,\ell}\right)\right)\right| \mid \boldsymbol{\pi}_0 = \boldsymbol{\psi}, \boldsymbol{\pi}'_0 = \boldsymbol{\psi}', D\right]\\
&\leq \frac{1}{g}\frac{1}{k}\sum_{\ell=1}^{g}\sum_{i=1}^{k}\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left|T(\mathsf{s}, D) - T(\mathsf{s}', D)\right|\mathbb{E}\left[N(\ell)\right]
\end{aligned}$$

Hence, it suffices to bound the quantity $\mathbb{E}[N(\ell)]$.

To that end, let $N_r(\ell)$ be the value of the smallest index m with $\overline{R}_m(\ell) \geq r$. We proceed analogously to standard analysis of the coupon collector's problem (see e.g., Section 2.2 of Levin and Peres, 2017). We can evaluate

$$\begin{aligned}
&P\left\{\overline{R}_m(\ell) \geq r+1 \mid \overline{R}_{m-1}(\ell) = r\right\}\\
&= \frac{1}{g}P\left\{\pi_\ell(I_m) \neq \pi'_\ell(I_m), \pi_\ell^{-1}(J_m) \neq \pi_\ell'^{-1}(J_m)\right\} = \frac{(n-r)^2}{gn^2}
\end{aligned}$$

and

$$P\left\{\overline{R}_m(\ell) < r \mid \overline{R}_{m-1}(\ell) = r\right\} = 0,$$

and thereby obtain the bound

$$\mathbb{E}[N(\ell)] = \sum_{r=1}^{n}\mathbb{E}\left[N_r(\ell) - N_{r-1}(\ell)\right] \leq \sum_{r=1}^{n}\frac{gn^2}{(n-r+1)^2} = gn^2\sum_{r=1}^{n}\frac{1}{r^2} \leq 2gn^2. \tag{E.29}$$

Hence, we find that (E.28) is upper bounded by

$$2gn^2\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}T(\mathsf{s}, D) - T(\mathsf{s}', D),$$

as required. ∎

E.8.2 Proof of Lemma E.2. Observe that

$$\frac{\mathrm{d}}{\mathrm{d}t} e^{tx} e^{(1-t)y} = (x-y)\, e^{tx} e^{(1-t)y}.$$

Thus, we find that

$$\begin{aligned}
c\,(e^x - e^y) &= c \int_0^1 \left(\frac{\mathrm{d}}{\mathrm{d}t} e^{tx} e^{(1-t)y} \right) \mathrm{dt} && \text{(Fundamental Theorem of Calculus)} \\
&= c\,(x-y) \int_0^1 e^{tx} e^{(1-t)y} \mathrm{dt} \\
&\leq c\,(x-y) \int_0^1 \left(t e^x + (1-t)\, e^y \right) && \text{(Convexity)} \\
&= \frac{c}{2}\,(x-y)\,(e^x + e^y) \\
&= \frac{1}{2} \left(\left(s^{-1} c^2\,(e^x + e^y) \right) \left(s\,(x-y)^2\,(e^x + e^y) \right) \right)^{1/2} \\
&\leq \frac{1}{4} \left(\left(s^{-1} c^2 \right) + s\,(x-y)^2 \right) (e^x + e^y)\,, && \text{(AM-GM)}
\end{aligned}$$

as required. ■

E.8.3 Proof of Lemma E.3. To begin, consider any collection of real numbers $x_1, \ldots, x_{2^c}$, for some positive integer c. For any integer $s > 0$, we have

$$\begin{aligned}
(x_1 \cdots x_{2^c})^{2s} &\leq \frac{1}{4} \left(\left(x_{i_1} \cdots x_{i_{2^{c-1}}} \right)^{2s} + \left(x_{i_{2^{c-1}+1}} \cdots x_{2^c} \right)^{2s} \right)^2 && \text{(Young's Inequality)} \\
&\leq \frac{1}{4} \left(\left(x_{i_1} \cdots x_{i_{2^{c-1}}} \right)^{2(s+1)} + 2\,(x_1 \cdots x_{2^c})^{2s} + \left(x_{i_{2^{c-1}+1}} \cdots x_{2^c} \right)^{2(s+1)} \right)
\end{aligned}$$

and so

$$(x_1 \cdots x_{2^c})^{2s} \leq \frac{1}{2} \left(x_{i_1} \cdots x_{i_{2^{c-1}}} \right)^{2(s+1)} + \frac{1}{2} \left(x_{i_{2^{c-1}+1}} \cdots x_{2^c} \right)^{2(s+1)}. \tag{E.30}$$

Consequently, we have that

$$x_1 \cdots x_{2^c} \leq \frac{1}{2^c} \sum_{i=1}^{2^c} x_i^{2c} \tag{E.31}$$

through 2^r applications of (E.30).

Now, to prove the Lemma, we may assume without loss that $h_i > 0$ for all i by continuity. Observe that

$$\mathbb{E}\left[\left(\sum_{m=0}^{\infty} X_m \right)^{2^c} \right] = \sum_{i_1=0}^{\infty} \cdots \sum_{i_{2^c}=0}^{\infty} \mathbb{E}\left[X_{i_1} \cdots X_{i_{2^c}} \right] \tag{E.32}$$

by dominated convergence. By writing

$$X_1 \cdots X_{2^c} = \prod_{j=1}^{2^c} \left(\frac{\prod_{k \neq j} h_k}{h_j^{2^{c-1}}} \right)^{1/2^c} X_j$$

we find that

$$\mathbb{E}\left[X_1 \cdots X_{2^c}\right] \leq \frac{1}{2^c} \sum_{j=1}^{2^c} \frac{\prod_{k \neq j} h_k}{h_j^{2^{c-1}}} h_j^{2^c} = \prod_{j=1}^{2^c} h_j$$

by (E.31). Hence, by (E.32), we have that

$$\mathbb{E}\left[\left(\sum_{m=0}^{\infty} X_m \right)^{2^c} \right] \leq \sum_{i_1=0}^{\infty} \cdots \sum_{i_{2^c}=0}^{\infty} \prod_{j=1}^{2^c} h_{i_j} = \left(\sum_{m=0}^{\infty} h_j \right)^{2^c},$$

as required. ■

E.8.4 Proof of Lemma E.4. We begin by constructing Stein representers $\tilde{V}(Z, Z')$ and $\check{V}(Z, Z')$ for the statistic $\tilde{v}_{g,k}(Z)$ and $\check{v}_{g,k}(Z)$, respectively. We will use the same exchangeable pair $(Z, Z')_{m \geq 0}$ and Markov chain $(Z_m, Z'_m)_{m \geq 1}$ defined in Section D.4. The subsequent result follows from an argument similar to Lemma D.1, again based on an idea expressed by Lemma 4.1 of Chatterjee (2005).

Lemma E.6.

(i) *Let ψ and ψ' be two sets, each containing g elements of $\mathcal{P}_n$. The inequalities*

$$\sum_{m=0}^{\infty} \left| \mathbb{E}\left[(\tilde{v}_{g,k}(Z_m) - \tilde{v}_{g,k}(Z'_m)) \mid Z_0 = Z, Z'_0 = Z' \right] \right| \leq n^2 \max_{\mathsf{s},\mathsf{s}' \in \mathsf{S}_{n,b}} \left(T(\mathsf{s}, D) - T(\mathsf{s}', D) \right)^2 \quad \textit{and}$$

$$\sum_{m=0}^{\infty} \left| \mathbb{E}\left[(\check{v}_{g,k}(Z_m) - \check{v}_{g,k}(Z'_m)) \mid Z_0 = Z, Z'_0 = Z' \right] \right| \leq 2gn^2 \max_{\mathsf{s} \in \mathsf{S}_{n,b}} \left(T(\mathsf{s}, D) - T(\mathsf{s}', D) \right)^2$$

hold almost surely.

(ii) *The functions*

$$\tilde{V}(Z, Z') = \sum_{m=0}^{\infty} \mathbb{E}\left[(\tilde{v}_{g,k}(Z_m) - \tilde{v}_{g,k}(Z'_m)) \mid Z_0 = Z, Z'_0 = Z' \right] \quad \textit{and}$$

$$\check{V}(Z, Z') = \sum_{m=0}^{\infty} \mathbb{E}\left[(\check{v}_{g,k}(Z_m) - \check{v}_{g,k}(Z'_m)) \mid Z_0 = Z, Z'_0 = Z' \right]$$

are finite and satisfy the equalities

$$\mathbb{E}\left[\tilde{V}(Z, Z') \mid Z \right] = \tilde{v}_{g,k}(Z) - v_{g,k}(D) \quad \textit{and}$$

$$\mathbb{E}\left[\check{V}(Z, Z') \mid Z \right] = \check{v}_{g,k}(Z) - v_{g,k}(D)$$

almost surely.

Next, we apply the concentration inequality stated in Theorem D.2, due to Chatterjee (2005, 2007). That is, to establish part (i) of the Lemma, it will suffice to characterize constants s and u that satisfy

$$U_{\tilde{v}}(Z) \leq s^{-1}u \quad \text{and} \quad U_{\tilde{V}}(Z) \leq su,$$

with probability $1-\delta$, where

$$U_{\tilde{v}}(Z) = \frac{1}{2}\mathbb{E}\left[\left(\tilde{v}(Z) - \tilde{v}(Z')\right) \mid Z\right] \quad \text{and} \quad U_{\tilde{V}}(Z) = \frac{1}{2}\mathbb{E}\left[\tilde{V}(Z,Z')^2 \mid Z\right].$$

The same statement holds for part (ii) of the Lemma, for the objects $U_{\check{v}}(Z)$ and $U_{\check{V}}(Z)$ defined analogously.

We obtain such a characterization through the application of Lemma D.3. To this end, observe that, by Lemma E.6, part (i), the bound

$$\left(\sum_{m=0}^{\infty} \mathbb{E}\left[\left(\tilde{v}_{g,k}(Z_m) - \tilde{v}_{g,k}(Z'_m)\right) \mid Z_0 = Z, Z'_0 = Z'\right]\right)^2 \tag{E.33}$$

$$\leq n^4 \max_{\mathsf{s},\mathsf{s}' \in \mathsf{S}_{n,b}} \left(T(\mathsf{s},D) - T(\mathsf{s}',D)\right)^4 \tag{E.34}$$

holds almost surely. The right hand side of (E.34) is square integrable, as the eighth-order split-stability $\zeta^{(8)}$ is finite almost surely. An analogous statement holds for the statistic $\check{v}_{g,k}(Z)$. Thus, deterministic bounds of the form (D.29) can be obtained through the application of the following Lemma.

Lemma E.7. *Suppose that Assumptions 4.1 and 4.2 hold and that the data D are independent and identically distributed. If the eighth-order split stability $\zeta^{(8)}$ is finite, then*
***(i)** The inequality*

$$\mathbb{E}\left[\mathbb{E}\left[\tilde{v}_{g,k}(Z_m) - \tilde{v}_{g,k}(Z'_m) \mid Z, Z'\right]^2 \mid \boldsymbol{\pi}\right] \lesssim \left(1 - \frac{2}{gn^2}\right)^{2m} \left(\frac{(2-\varphi k-\varphi)^4}{n^2 g^4}\right) \Gamma^{(2)}_{k,\varphi,b},$$

holds almost surely for all integers $m \geq 0$, and
***(ii)** The inequality*

$$\mathbb{E}\left[\mathbb{E}\left[\check{v}_{g,k}(Z_m) - \check{v}_{g,k}(Z'_m) \mid Z, Z'\right]^2 \mid \boldsymbol{\pi}\right] \lesssim \left(1 - \frac{2}{gn^2}\right)^{2m} \left(\frac{(2-\varphi k-\varphi)^4}{n^2 g^3}\right) \Gamma^{(2)}_{k,\varphi,b},$$

holds almost surely for all integers $m \geq 0$.

Thus, by Lemma D.3, part (i), the inequalities

$$U_{\tilde{V}}(Z) \lesssim \frac{1}{\delta}\left(\frac{gn^2}{2}\right)^2 \left(\frac{(2-\varphi k-\varphi)^4}{n^2 g^4}\right) \Gamma^{(2)}_{k,\varphi,b}$$

$$\lesssim \left(\frac{gn^2}{2}\right)\left(\frac{1}{\delta}\frac{(2-\varphi k-\varphi)^4}{g^3}\right)\Gamma^{(2)}_{k,\varphi,b}$$

and

$$U_{\tilde{v}}(Z) \lesssim \frac{1}{\delta}\left(\frac{(2-\varphi k-\varphi)^4}{n^2 g^4}\right)\Gamma^{(2)}_{k,\varphi,b}$$
$$\lesssim \left(\frac{2}{gn^2}\right)\left(\frac{1}{\delta}\frac{(2-\varphi k-\varphi)^4}{g^3}\right)\Gamma^{(2)}_{k,\varphi,b}$$

both hold with probability greater than $1-\delta$. Hence, we obtain the bound (E.16) by applying Theorem D.2 and choosing $s = gn^2/2$ and

$$u = \frac{1}{\delta}\frac{(2-\varphi k-\varphi)^4}{g^3}\Gamma^{(2)}_{k,\varphi,b}\,.$$

Analogous inequalities for the objects $U_{\check{v}}(Z)$ and $U_{\check{V}}(Z)$ hold by Lemma D.3, part (ii), where in that case

$$u = \frac{1}{\delta}\frac{(2-\varphi k-\varphi)^4}{g^2}n^4\Gamma^{(2)}_{k,\varphi,b}\,.$$

which similarly implies the bound (E.17) by Theorem D.2. ■

E.8.5 Proof of Lemma E.6. Reinstate the notation of the proof of Lemma E.1. We begin by noting that

$$\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left(T(\mathsf{s},D)-T(\mathsf{s}',D)\right)^2 = \max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left(T(\mathsf{s},D)-\overline{a}(D)\right)^2+\left(T(\mathsf{s}',D)-\overline{a}(D)\right)^2$$
$$+2\left(T(\mathsf{s},D)-\overline{a}(D)\right)\left(T(\mathsf{s}',D)-\overline{a}(D)\right)$$
$$\geq 4\max_{\mathsf{s}\in\mathsf{S}_{n,b}}\left(T(\mathsf{s},D)-\overline{a}(D)\right)^2.$$

Observe that

$$\sum_{i,i'=1}^{k}\left(T_i(\pi_{m,\ell})-\overline{a}(D)\right)\left(T_i(\pi_{m,\ell})-\overline{a}(D)\right)-\sum_{i,i'=1}^{k}\left(T_i\left(\pi'_{m,\ell}\right)-\overline{a}(D)\right)\left(T_{i'}\left(\pi'_{m,\ell}\right)-\overline{a}(D)\right)=0$$

for all for all $m'\geq m$ if and only if $\overline{R}_m(\ell)=n$. Thus, we have that

$$\sum_{m=0}^{\infty}\left|\mathbb{E}\left[\tilde{v}_{g,k}(Z_m)-\tilde{v}_{g,k}(Z'_m)\mid Z_0=\left(\mathsf{r}(\boldsymbol{\psi}),D\right),Z'_0=\left(\mathsf{r}(\boldsymbol{\psi}'),D\right)\right]\right|$$
$$\leq\sum_{m=0}^{\infty}\frac{1}{g^2k^2}\sum_{\ell=1}^{g}\sum_{i,i'=1}^{k}\mathbb{E}\Bigg[\Bigg|\left(T_i(\pi_{m,\ell})-\overline{a}(D)\right)\left(T_{i'}(\pi_{m,\ell})-\overline{a}(D)\right)$$
$$-\left(T_i\left(\pi'_{m,\ell}\right)-\overline{a}(D)\right)\left(T_{i'}\left(\pi'_{m,\ell}\right)-\overline{a}(D)\right)\Bigg|\mid Z_0=\left(\mathsf{r}(\boldsymbol{\psi}),D\right),Z'_0=\left(\mathsf{r}(\boldsymbol{\psi}'),D\right)\Bigg]$$

$$\leq \frac{2}{g^2k^2}\sum_{\ell=1}^{g}\sum_{i,i'=1}^{k}\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left|\left(T\left(\mathsf{s},D\right)-\overline{a}\left(D\right)\right)\left(T\left(\mathsf{s}',D\right)-\overline{a}\left(D\right)\right)\right|\mathbb{E}\left[N\left(\ell\right)\right].$$

$$\leq \frac{2}{g}\max_{\mathsf{s}\in\mathsf{S}_{n,b}}\left(T(\mathsf{s},D)-\overline{a}\left(D\right)\right)^2\mathbb{E}\left[N\left(\ell\right)\right].$$

$$\leq \frac{1}{2g}\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left(T(\mathsf{s},D)-T(\mathsf{s}',D)\right)^2\mathbb{E}\left[N\left(\ell\right)\right].$$

Similarly, we have that

$$\sum_{m=0}^{\infty}\left|\mathbb{E}\left[\check{v}_{g,k}(Z_m)-\check{v}_{g,k}(Z_m')\mid Z_0=\left(\mathsf{r}\left(\boldsymbol{\psi}\right),D\right),Z_0'=\left(\mathsf{r}\left(\boldsymbol{\psi}'\right),D\right)\right]\right|$$

$$\leq \sum_{m=0}^{\infty}\frac{1}{g^2k^2}\sum_{\ell,\ell'=1}^{g}\sum_{i,i'=1}^{k}\mathbb{E}\Bigg[\Big|\left(T_i\left(\pi_{m,\ell}\right)-\overline{a}\left(D\right)\right)\left(T_{i'}\left(\pi_{m,\ell'}\right)-\overline{a}\left(D\right)\right)$$

$$-\left(T_i\left(\pi_{m,\ell}'\right)-\overline{a}\left(D\right)\right)\left(T_{i'}\left(\pi_{m,\ell'}'\right)-\overline{a}\left(D\right)\right)\Big|\mid Z_0=\left(\mathsf{r}\left(\boldsymbol{\psi}\right),D\right),Z_0'=\left(\mathsf{r}\left(\boldsymbol{\psi}'\right),D\right)\Bigg]$$

$$\leq \frac{2}{g^2k^2}\sum_{\ell,\ell'=1}^{g}\sum_{i,i'=1}^{k}\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left|\left(T\left(\mathsf{s},D\right)-\overline{a}\left(D\right)\right)\left(T\left(\mathsf{s}',D\right)-\overline{a}\left(D\right)\right)\right|\mathbb{E}\left[\max\left\{N\left(\ell\right),N\left(\ell'\right)\right\}\right]$$

$$\leq \frac{2}{g^2k^2}\sum_{\ell,\ell'=1}^{g}\sum_{i,i'=1}^{k}\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left|\left(T\left(\mathsf{s},D\right)-\overline{a}\left(D\right)\right)\left(T\left(\mathsf{s}',D\right)-\overline{a}\left(D\right)\right)\right|\mathbb{E}\left[N\left(\ell\right)+N\left(\ell'\right)\right]$$

$$\leq \frac{1}{2}\max_{\mathsf{s},\mathsf{s}'\in\mathsf{S}_{n,b}}\left(T(\mathsf{s},D)-T(\mathsf{s}',D)\right)^2\left|\mathbb{E}\left[N\left(\ell\right)+N\left(\ell'\right)\right]\right.$$

Thus, part (i) of the Lemma follows by the bound (E.29). Part (ii) of the Lemma then follows by an argument analogous to the proof of Lemma D.1. ■

E.8.6 Proof of Lemma E.7. We reinstate the notation introduced in the proof of Lemma D.4 from Section E.4. First, observe that

$$\begin{aligned}
&\mathbb{E}\left[\mathbb{E}\left[\tilde{v}_{g,k}(Z_m)-\tilde{v}_{g,k}(Z_m')\mid Z,Z'\right]^2\mid\boldsymbol{\pi}\right]\\
&=\mathbb{E}\left[\left(P\left\{\mathcal{H}_m\right\}\mathbb{E}\left[\tilde{v}_{g,k}(Z_m)-\tilde{v}_{g,k}(Z_m')\mid\mathcal{H}_m,Z,Z'\right]\right)^2\mid\boldsymbol{\pi}\right]\\
&\leq\left(1-\frac{2}{gn^2}\right)^{2m}\left(\frac{2kb\left(2n-bk-b\right)}{n^2}\right)^2\mathbb{E}\left[\left(\tilde{v}_{g,k}(Z_m)-\tilde{v}_{g,k}(Z_m')\right)^2\mid\mathcal{H}_m,\boldsymbol{\pi}\right]
\end{aligned}\tag{E.35}$$

as before. Recall the notation

$$\overline{a}(\mathsf{r}_\ell,D)=\frac{1}{k}\sum_{i=1}^{k}(T(\mathsf{s}_{\ell,i},D)-\overline{a}(D))$$

and observe that

$$
\begin{aligned}
&\mathbb{E}\left[\left(\tilde{v}_{g,k}(Z_m)-\tilde{v}_{g,k}(Z'_m)\right)^2 \mid \mathcal{H}_m, \boldsymbol{\pi}\right] \\
&= \frac{1}{g^4}\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)^2-\overline{a}(\mathsf{r}(\pi'_{m,L}),D)^2\right)^2 \mid \mathcal{H}_m\right] \\
&= \frac{1}{g^4}\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)+\overline{a}(\mathsf{r}(\pi'_{m,L}),D)\right)^2\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)-\overline{a}(\mathsf{r}(\pi'_{m,L}),D)\right)^2 \mid \mathcal{H}_m\right] \\
&\leq \frac{1}{g^4}\left(\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)+\overline{a}(\mathsf{r}(\pi'_{m,L}),D)\right)^4 \mid \mathcal{H}_m\right]\right)^{1/2} && \text{(Cauchy-Schwarz)} \\
&\quad\cdot\left(\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)-\overline{a}(\mathsf{r}(\pi'_{m,L}),D)\right)^4 \mid \mathcal{H}_m\right]\right)^{1/2} \\
&\leq \frac{2^4}{g^4}\left(\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)-\overline{a}(D)\right)^4\right]\right)^{1/2} && \text{(Hölder)} \\
&\quad\cdot\left(\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)-\overline{a}(\mathsf{r}(\pi'_{m,L}),D)\right)^4 \mid \mathcal{H}_m\right]\right)^{1/2} . && \text{(E.36)}
\end{aligned}
$$

Observe that

$$
\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)-\overline{a}(D)\right)^4\right] \leq 3^2\left(2^4(2-\varphi k-\varphi)^2\right)^2\Gamma^{(2)}_{k,\varphi,b}
$$

by Theorem D.2, as Assumption 4.1 is maintained and the eighth-order sample-split stability $\zeta^{(8)}$ is finite. In turn, we have that

$$
\mathbb{E}\left[\left(\overline{a}(\mathsf{r}(\pi_{m,L}),D)-\overline{a}(\mathsf{r}(\pi'_{m,L}),D)\right)^4 \mid \mathcal{H}_m\right] \leq \frac{4}{k^4b^4}\Gamma^{(2)}_{k,\varphi,b} \tag{E.37}
$$

by (E.7), (E.13), and (E.14). Hence, we have that

$$
\mathbb{E}\left[\left(\tilde{v}_{g,k}(Z_m)-\tilde{v}_{g,k}(Z'_m)\right)^2 \mid \mathcal{H}_m, \boldsymbol{\pi}\right] \leq \frac{3\cdot 2^9}{k^2b^2g^4}(2-\varphi k-\varphi)^2\Gamma^{(2)}_{k,\varphi,b} . \tag{E.38}
$$

Combining (E.35), (E.37), (E.38), we find that

$$
\mathbb{E}\left[\mathbb{E}\left[\tilde{v}_{g,k}(Z_m)-\tilde{v}_{g,k}(Z'_m) \mid Z, Z'\right]^2 \mid \boldsymbol{\pi}\right] \leq \left(1-\frac{2}{gn^2}\right)^{2m}\left(\frac{\left(3\cdot 2^{11}\right)(2-\varphi k-\varphi)^4}{n^2g^4}\right)\Gamma^{(2)}_{k,\varphi,b} ,
$$

which completes the proof of the first part of the Lemma.

Second, following the same argument, we again have that

$$
\begin{aligned}
&\mathbb{E}\left[\mathbb{E}\left[\check{v}_{g,k}(Z_m)-\check{v}_{g,k}(Z'_m) \mid Z, Z'\right]^2 \mid \boldsymbol{\pi}\right] \\
&\leq \left(1-\frac{2}{gn^2}\right)^{2m}\left(\frac{2kb\,(2n-bk-b)}{n^2}\right)^2\mathbb{E}\left[\left(\check{v}_{g,k}(Z_m)-\check{v}_{g,k}(Z'_m)\right)^2 \mid \mathcal{H}_m, \boldsymbol{\pi}\right] && \text{(E.39)}
\end{aligned}
$$

In this case, we can compute

$$
\mathbb{E}\left[\left(\check{v}_{g,k}(Z_m)-\check{v}_{g,k}(Z'_m)\right)^2 \mid \mathcal{H}_m, \boldsymbol{\pi}\right]
$$

$$
\begin{aligned}
&= \mathbb{E}\left[\left(\left(a(Z_m)-\overline{a}(D)\right)^2-\left(a(Z'_m)-\overline{a}(D)\right)^2\right)^2 \mid \mathcal{H}_m\right] \\
&= \mathbb{E}\left[\left(a(Z_m)-\overline{a}(D)+a(Z'_m)-\overline{a}(D)\right)^2\left(a(Z_m)-a(Z'_m)\right)^2 \mid \mathcal{H}_m\right] \\
&\leq \left(\mathbb{E}\left[\left(a(Z_m)-\overline{a}(D)+a(Z'_m)-\overline{a}(D)\right)^4 \mid \mathcal{H}_m\right]\right)^{1/2} \qquad \text{(Cauchy-Schwarz)} \\
&\quad \cdot \left(\mathbb{E}\left[\left(a(Z_m)-a(Z'_m)\right)^4 \mid \mathcal{H}_m\right]\right)^{1/2} \\
&\leq 2^4\left(\mathbb{E}\left[\left(a(Z_m)-\overline{a}(D)\right)^4\right]\right)^{1/2}\left(\mathbb{E}\left[\left(a(Z_m)-a(Z'_m)\right)^4 \mid \mathcal{H}_m\right]\right)^{1/2}, \qquad \text{(E.40)}
\end{aligned}
$$

where the last inequality follows from Hölder's inequality. Again we have that

$$
\mathbb{E}\left[\left(a(Z_m)-a(Z'_m)\right)^4\right] \leq 3^2\left(\frac{2^4\varphi^2(2-\varphi k-\varphi)^2}{g}\right)^2\Gamma^{(2)}_{k,\varphi,b} \qquad \text{(E.41)}
$$

by Theorem D.2, as Assumption 4.1 is maintained and the eighth-order sample-split stability $\zeta^{(8)}$ is finite. Similarly. we have that

$$
\mathbb{E}\left[\left(a(Z_m)-\overline{a}(D)\right)^4 \mid \mathcal{H}_m\right] \leq \frac{4}{g^4k^4b^4}\Gamma^{(2)}_{k,\varphi,b} \qquad \text{(E.42)}
$$

by (E.7), (E.13), and (E.14). Combining (E.39), (E.41), (E.42), we find that

$$
\mathbb{E}\left[\left(\check{v}_{g,k}(Z_m)-\check{v}_{g,k}(Z'_m)\right)^2 \mid \mathcal{H}_m,\boldsymbol{\pi}\right] \leq \left(1-\frac{2}{gn^2}\right)^{2m}\left(\frac{\left(3\cdot 2^9\right)\varphi^4\left(2-\varphi k-\varphi\right)^4}{n^2g^3}\right)\Gamma^{(2)}_{k,\varphi,b},
$$

which completes the proof of the second part of the Lemma. ■

E.8.7 Proof of Lemma E.5, Part (i). Observe that

$$
\begin{aligned}
&P\left\{|U(\mathsf{R}_{\hat{g},k},D)| \geq t\sqrt{v_{g^\star,k}(D)}, |\hat{g}-g^\star| \leq cg^\star \mid D\right\} \\
&= P\left\{\sum_{i=1}^{g}\overline{a}\left(\mathsf{r}_{i,k},D\right)-\sum_{i=1}^{g^\star}\overline{a}\left(\mathsf{r}_{i,k},D\right) \geq tg^\star\sqrt{v_{g^\star,k}(D)}, |\hat{g}-g^\star| \leq cg^\star \mid D\right\} \\
&\leq P\left\{\max_{g^\star(1-c)\leq g\leq g^\star}\left|\sum_{i=1}^{g}\overline{a}\left(\mathsf{r}_{i,k},D\right)-\sum_{i=1}^{g^\star}\overline{a}\left(\mathsf{r}_{i,k},D\right)\right| \geq tg^\star\sqrt{v_{g^\star,k}(D)} \mid D\right\} \\
&+ P\left\{\max_{g^\star\leq g\leq g^\star(1+c)}\left|\sum_{i=1}^{g}\overline{a}\left(\mathsf{r}_{i,k},D\right)-\sum_{i=1}^{g^\star}\overline{a}\left(\mathsf{r}_{i,k},D\right)\right| \geq tg^\star\sqrt{v_{g^\star,k}(D)} \mid D\right\} \\
&= P\left\{\max_{g^\star(1-c)\leq g\leq g^\star}\left|\sum_{i=1}^{g^\star-g}\overline{a}\left(\mathsf{r}_{i,k},D\right)\right| \geq tg^\star\sqrt{v_{g^\star,k}(D)} \mid D\right\} \\
&+ P\left\{\max_{g^\star\leq g\leq g^\star(1+c)}\left|\sum_{i=1}^{g-g^\star}\overline{a}\left(\mathsf{r}_{i,k},D\right)\right| \geq tg^\star\sqrt{v_{g^\star,k}(D)} \mid D\right\}. \qquad \text{(E.43)}
\end{aligned}
$$

To bound the two probabilities (E.43), we apply the following Chernoff-type variation to the Kolmogorov maximal inequality, due to Steiger (1970).

Theorem E.2 (Steiger, 1970)**.** *Let S_i, $i = 1, 2, \ldots$, be a real-valued martingale sequence. If the moment generating function*

$$m_n(\theta) = \mathbb{E}\left[\exp\left(\theta S_n\right)\right]$$

is finite for all positive θ, then the inequality

$$\log\ P\left\{\max_{1\leq n'\leq n} S_{n'} > t\right\} \leq \inf_{\theta>0}\left(\log m_n(\theta) - \theta t\right),$$

holds.

Conditional on D, the random variables

$$\overline{a}\left(\mathsf{r}_{i,k}, D\right), \quad i = 1, 2, \ldots,$$

are mean-zero, independent, and identically distributed. Thus, the partial sums

$$S_m = \sum_{i=1}^{m} \overline{a}\left(\mathsf{r}_{i,k}, D\right)$$

are a martingale sequence. Moreover, though inspection of the proof of Lemma D.2, we find that Theorem Corollary D.1 implies that

$$\begin{aligned}
&\inf_{\theta>0}\left(\log \mathbb{E}\left[\exp\left(\theta S_{\lfloor cg^\star\rfloor}\right) \mid D\right] - \theta\tau\right) \\
&= \inf_{\theta>0}\left(\log \mathbb{E}\left[\exp\left(\frac{\theta}{\lfloor cg^\star\rfloor} S_{\lfloor cg^\star\rfloor}\right) \mid D\right] - \theta\frac{\tau}{\lfloor cg^\star\rfloor}\right) \\
&\leq -\frac{\lfloor cg^\star\rfloor}{2^4(2-\varphi k-\varphi)^2\Gamma^{(1)}_{k,\varphi,b}} \frac{\delta\tau^2}{\left(\lfloor cg^\star\rfloor\right)^2} \\
&\leq -\frac{\delta}{2^4(2-\varphi k-\varphi)^2\Gamma^{(1)}_{k,\varphi,b}} \frac{\tau^2}{cg^\star}
\end{aligned}$$

with probability greater than $1-\delta$, as Assumption 4.1 holds and the fourth-order split stability $\zeta^{(4)}$ is finite. Thus, by setting

$$\tau = tg^\star\sqrt{v_{g^\star,k}(D)} = \sqrt{g^\star}t\left(v_{1,k}(D)\right)^{1/2}$$

we find that

$$\begin{aligned}
&\log\frac{1}{2}P\left\{|U(\mathsf{R}_{\hat{g},k}, D)| \geq t\sqrt{v_{g^\star,k}(D)}, |\hat{g}-g^\star| \leq cg^\star \mid D\right\} \\
&\leq -\frac{\delta v_{1,k}(D)}{2^4(2-\varphi k-\varphi)^2\Gamma^{(1)}_{k,\varphi,b}} \frac{t^2}{c}
\end{aligned}$$

with probability greater than $1-\delta$, by Theorem E.2 and the inequality (E.43).

E.8.8 Proof of Lemma E.5, Part (ii). Observe that

$$P\left\{|\hat{g}-g^\star| > cg^\star \mid D\right\} = P\left\{g^\star(1+c) < \hat{g} \mid D\right\} + P\left\{\hat{g} < g^\star(1-c) \mid D\right\}. \tag{E.44}$$

We begin by handling the first term. We have that

$$\begin{aligned}
&P\left\{g^\star(1+c) < \hat{g} \mid D\right\} \\
&\leq P\left\{\hat{v}_{g^\star(1+c),k}(Z) - v_{g^\star(1+c),k}(D) + v_{g^\star(1+c),k}(D) > \frac{1}{2}\left(\frac{\xi}{z_{1-\beta/2}}\right)^2 \mid D\right\} \\
&\leq P\left\{\hat{v}_{g^\star(1+c),k}(Z) - v_{g^\star(1+c),k}(D) > \frac{v_{1,k}(D)}{g^\star} - \frac{v_{1,k}(D)}{g^\star(1+c)} \mid D\right\} \\
&= P\left\{\hat{v}_{g^\star(1+c),k}(Z) - v_{g^\star(1+c),k}(D) > \frac{v_{1,k}(D)}{g^\star}\frac{c}{1+c} \mid D\right\},
\end{aligned}$$

where the first inequality follows the definition of $g^\star$. Thus, as Assumption 4.1 holds and the eighth-order split stability $\zeta^{(8)}$ is finite, we have that

$$\begin{aligned}
\log\frac{1}{4}P\left\{g^\star(1+c) < \hat{g} \mid D\right\} &\lesssim -\frac{\delta(v_{1,k}(D))^2}{(2-\varphi k-\varphi)^4}\frac{g^\star(1+c)c^2}{\Gamma^{(2)}_{k,\varphi,b}} \\
&\lesssim -\frac{\delta(v_{1,k}(D))^3}{(2-\varphi k-\varphi)^4}\frac{z^2_{1-\beta/2}c^2}{\xi^2\Gamma^{(2)}_{k,\varphi,b}}
\end{aligned}$$

with probability greater than $1-\delta$, by Lemma D.5, the definition of $g^\star$ and the assumption that $0 < c < 1/2$.

Next, we bound the second term in (E.44). Define the partial sums

$$A_g = \sum_{\ell=1}^{g}\left(\frac{1}{k^2}\sum_{i,i'=1}^{k}\left(T(\mathsf{s}_{\ell,i},D)-\overline{a}(D)\right)\left(T(\mathsf{s}_{\ell,i'},D)-\overline{a}(D)\right) - v_{1,k}(D)\right) \quad \text{and}$$

$$\begin{aligned}
B_g = \sum_{\ell=1}^{g}\Bigg(&\frac{1}{k^2}\sum_{i,i'=1}^{k}\left(T(\mathsf{s}_{\ell,i},D)-\overline{a}(D)\right)\left(T(\mathsf{s}_{\ell,i'},D)-\overline{a}(D)\right) \\
&+ 2\sum_{\ell'=1}^{\ell-1}\left(T(\mathsf{s}_{\ell,i},D)-\overline{a}(D)\right)\left(T(\mathsf{s}_{\ell',i'},D)-\overline{a}(D)\right) - v_{1,k}(D)\Bigg).
\end{aligned}$$

Observe that the equality

$$\hat{v}_{g,k}(Z) - v_{g,k}(D) = \frac{g}{g-1}\left(\tilde{v}_{g,k}(Z) - v_{g,k}(D)\right) - \frac{1}{g-1}\left(\check{v}_{g,k}(Z) - v_{g,k}(D)\right),$$

from the proof of Lemma D.5, implies that

$$\begin{aligned}\hat{v}_{g,k}(Z) - v_{g,k}(D) &= \frac{1}{g(g-1)} \sum_{\ell=1}^{g} \frac{1}{k^2} \sum_{i,i'=1}^{k} (T(\mathsf{s}_{\ell,i}, D) - a(Z))(T(\mathsf{s}_{\ell,i'}, D) - a(Z)) - \frac{v_{1,k}(D)}{g} \\ &= \frac{1}{g-1}\frac{1}{g} A_g - \frac{1}{g-1}\frac{1}{g^2} B_g\end{aligned}$$

for all positive g. Thus, we can write

$$\begin{aligned}&P\{\hat{g} < g^\star(1-c) \mid D\} \\ &= P\left\{ \min_{2 \le g' \le g^\star(1-c)} \hat{v}_{g',k}(Z) \le \left(\frac{\xi}{z_{1-\beta/2}}\right)^2 \mid D \right\} \\ &= P\left\{ \min_{2 \le g' \le g^\star(1-c)} \frac{(g' A_{g'} - B_{g'})}{(g'-1)(g')^2} + \frac{1}{g'} v_{1,k}(D) \le \left(\frac{\xi}{z_{1-\beta/2}}\right)^2 \mid D \right\},\end{aligned}$$

where the first equality follows from the definition of $\hat{g}$. Now, in the event that

$$\min_{2 \le g' \le g^\star(1-c)} \frac{(g' A_{g'} - B_{g'})}{(g'-1)(g')^2} + \frac{1}{g'} v_{1,k}(D) \le \left(\frac{\xi}{z_{1-\beta/2}}\right)^2, \tag{E.45}$$

it must also be the case that

$$\min_{2 \le g' \le g^\star(1-c)} (g'-1)(g')^2 \left(\frac{(g' A_{g'} - B_{g'})}{(g'-1)(g')^2} + \frac{1}{g'} v_{1,k}(D) \right) \le (\hat{g}-1)(\hat{g})^2 \left(\frac{\xi}{z_{1-\beta/2}}\right)^2 \tag{E.46}$$

as $\hat{g} \le g^\star(1-c)$ necessarily. But then, similarly, (E.46) implies that

$$\min_{2 \le g' \le g^\star(1-c)} (g' A_{g'} - B_{g'}) + \frac{(\hat{g}-1)(\hat{g})^2}{g'} v_{1,k}(D) \le (\hat{g}-1)(\hat{g})^2 \left(\frac{\xi}{z_{1-\beta/2}}\right)^2,$$

and in turn

$$\begin{aligned}&\min_{2 \le g' \le g^\star(1-c)} \frac{(g' A_{g'} - B_{g'})}{(g^\star(1-c)-1)(g^\star(1-c))^2} \\ &\le \frac{(\hat{g}-1)(\hat{g})^2}{(g^\star(1-c)-1)(g^\star(1-c))^2} \left(\frac{1}{g^\star - 1} - \frac{1}{g^\star(1-c)} \right) v_{1,k}(D) \\ &= \frac{(\hat{g}-1)(\hat{g})^2}{(g^\star(1-c)-1)(g^\star(1-c))^2} \left(\frac{1 - g^\star c}{g^\star(g^\star-1)(1-c)} \right) v_{1,k}(D),\end{aligned}$$

are then also true. Finally, again as (E.45) is equivalent to $\hat{g} < g^\star(1-c)$, we have that

$$\begin{aligned}&P\left\{ \min_{2 \le g' \le g^\star(1-c)} \frac{(g' A_{g'} - B_{g'})}{(g'-1)(g')^2} + \frac{1}{g'} v_{1,k}(D) \le \left(\frac{\xi}{z_{1-\beta/2}}\right)^2 \mid D \right\} \\ &\le P\left\{ \min_{2 \le g' \le g^\star(1-c)} \frac{g' A_{g'} - B_{g'}}{(g^\star(1-c)-1)(g^\star(1-c))^2} \le \left(\frac{1 - g^\star c}{g^\star(g^\star-1)(1-c)} \right) v_{1,k}(D) \mid D \right\}.\end{aligned}$$

Now, observe that we can write

$$P\left\{\min_{2\leq g'\leq g^\star(1-c)}\frac{g'A_{g'}-B_{g'}}{\left(g^\star\left(1-c\right)-1\right)\left(g^\star\left(1-c\right)\right)^2}\leq\left(\frac{1-g^\star c}{g^\star\left(g^\star-1\right)\left(1-c\right)}\right)v_{1,k}(D)\mid D\right\}$$
$$=P\left\{\max_{2\leq g'\leq g^\star(1-c)}\frac{B_{g'}-g'A_{g'}}{\left(g^\star\left(1-c\right)-1\right)\left(g^\star\left(1-c\right)\right)^2}\geq\left(\frac{g^\star c-1}{g^\star\left(g^\star-1\right)\left(1-c\right)}\right)v_{1,k}(D)\mid D\right\}.$$

We bound this term by combining the argument used to establish Lemma D.5 with an application of Theorem E.2. To this end, observe that

$$\begin{aligned}
&P\left\{\max_{2\leq g'\leq g}\frac{B_{g'}-g'A_{g'}}{\left(g-1\right)g^2}\leq t\mid D\right\}\\
&\geq P\left\{\max_{2\leq g'\leq g}\frac{-1}{g-1}\frac{g'}{g^2}A_{g'}\leq\frac{1}{1+\sqrt{g}}t\mid D\right\}+P\left\{\max_{2\leq g'\leq g}\frac{1}{g-1}\frac{1}{g^2}B_{g'}\leq\frac{\sqrt{g}}{1+\sqrt{g}}t\mid D\right\}-1\\
&\geq P\left\{\max_{2\leq g'\leq g}\frac{g}{g-1}\frac{-1}{g^2}A_{g'}\leq\frac{\sqrt{g}}{1+\sqrt{g}}t\mid D\right\}+P\left\{\max_{2\leq g'\leq g}\frac{1}{g-1}\frac{1}{g^2}B_{g'}\leq\frac{1}{1+\sqrt{g}}t\mid D\right\}-1\\
&\geq P\left\{\max_{2\leq g'\leq g}-A_{g'}\leq g^2\frac{1}{\sqrt{g}}\frac{g-1}{1+\sqrt{g}}t\mid D\right\}+P\left\{\max_{2\leq g'\leq g}|B_{g'}|\leq g^2\frac{g-1}{1+\sqrt{g}}t\mid D\right\}-1 \qquad \text{(E.47)}
\end{aligned}$$

for any $t>0$ and any positive integer D. Observe that the partial sums A_g and B_g are both martingale sequences. As Assumption 4.1 holds and the eighth-order split stability $\zeta^{(8)}$ is finite, though inspection of the proof of Lemma D.2, Lemma E.4 implies that implies that

$$\begin{aligned}
&\inf_{\theta>0}\left(\log\mathbb{E}\left[\exp\left(\theta A_g\right)\mid D\right]-\theta g^2\frac{1}{\sqrt{g}}\frac{g-1}{1+\sqrt{g}}t\right)\\
&=\inf_{\theta>0}\left(\log\mathbb{E}\left[\exp\left(\frac{\theta}{g^2}A_g\right)\mid D\right]-\theta\frac{1}{\sqrt{g}}\frac{g-1}{1+\sqrt{g}}t\right)\\
&\lesssim-\frac{\delta}{(2-\varphi k-\varphi)^4}\frac{g^3t^2}{\Gamma^{(2)}_{k,\varphi,b}} \qquad \text{(E.48)}
\end{aligned}$$

and

$$\begin{aligned}
&\inf_{\theta>0}\left(\log\mathbb{E}\left[\exp\left(\theta B_g\right)\mid D\right]-\theta g^2\frac{g-1}{1+\sqrt{g}}t\right)\\
&=\inf_{\theta>0}\left(\log\mathbb{E}\left[\exp\left(\frac{\theta}{g^2}B_g\right)\mid D\right]-\theta\frac{g-1}{1+\sqrt{g}}t\right)\\
&\lesssim-\frac{\delta}{(2-\varphi k-\varphi)^4}\frac{g^3t^2}{\Gamma^{(2)}_{k,\varphi,b}} \qquad \text{(E.49)}
\end{aligned}$$

each with probability greater than $1-\delta$, where we have used the facts that $4g\leq\left(1+\sqrt{g}\right)^2$ for all $g\geq1$ and $(1/4)\,g^2\geq(g-1)^2$ for all $g\geq2$. Hence, by Theorem E.2, and plugging (E.48) and

(E.49) into (E.47), we find that

$$\log \frac{1}{4} P\left\{\max_{2 \leq g' \leq g} \frac{B_{g'} - g' A_{g'}}{(g'-1)\,(g')^2} \geq t \mid D\right\} \lesssim -\frac{\delta}{(2-\varphi k-\varphi)^4} \frac{g^3 t^2}{\Gamma^{(2)}_{k,\varphi,b}}$$

with probability greater than $1-\delta$. Consequently, by the definition of $g^\star$, we find that

$$\begin{aligned}
&\log \frac{1}{4} P\left\{g^\star - \hat{g} \geq c \mid D\right\} \\
&= \log \frac{1}{4} P\left\{\max_{2 \leq g' \leq g^\star(1-c)} \frac{B_{g'} - g' A_{g'}}{(g^\star(1-c)-1)\,(g^\star(1-c))^2} \geq \left(\frac{g^\star c - 1}{g^\star\,(g^\star-1)\,(1-c)}\right) v_{1,k}(D) \mid D\right\} \\
&\lesssim -\frac{\delta (v_{1,k}(D))^2}{(2-\varphi k-\varphi)^4} \frac{g^\star (1-c)(g^\star c-1)^2}{(g^\star-1)^2 \Gamma^{(2)}_{k,\varphi,b}} \\
&\lesssim -\frac{\delta (v_{1,k}(D))^2}{(2-\varphi k-\varphi)^4} \frac{g^\star c^2}{\Gamma^{(2)}_{k,\varphi,b}} \\
&\lesssim -\frac{\delta (v_{1,k}(D))^3}{(2-\varphi k-\varphi)^4} \frac{z^2_{1-\beta/2} c^2}{\xi^2 \Gamma^{(2)}_{k,\varphi,b}}
\end{aligned}$$

where in the second to last inequality we have used the facts that $\frac{1}{2}x \leq x-1$ for $x \geq 2$ and $g^\star c \geq 2$. Thus, putting the pieces together, we find that

$$\log \frac{1}{8} P\left\{|\hat{g} - g^\star| > c g^\star \mid D\right\} \lesssim -\frac{\delta (v_{1,k}(D))^3}{(2-\varphi k-\varphi)^4} \frac{z^2_{1-\beta/2} c^2}{\xi^2 \Gamma^{(2)}_{k,\varphi,b}}$$

with probability greater than $1-\delta$, as required. ■

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