Supplementary Materials for "Auditing ML Models for Individual Bias and Unfairness"

A Proofs

A.1 Proof of Proposition in Section 2

Proof of Proposition 2.2. For the simplicity of notations, we drop the subscript of the loss function picked by the auditor, that is, we denote ℓ_h by ℓ. Furthermore, let

$$\ell_\lambda^c(z) = \ell_\lambda^c(x,y) \triangleq \sup_{x_2\in\mathcal{X}} \{\ell(x_2,y) - \lambda c((x,y),(x_2,y))\}.$$

By the duality result of Blanchet and Murthy (2019), for any $\varepsilon > 0$, we have

$$\sup_{P:W(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] = \inf_{\lambda\ge 0}\{\lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_\lambda^c(Z)]\}$$

and

$$\sup_{P:W_*(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] = \inf_{\lambda\ge 0}\{\lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_\lambda^{c_*}(Z)]\}.$$

Let $\lambda_* \in \arg\min_{\lambda\ge 0}\{\lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_\lambda^{c_*}(Z)]\}$. Then we have

$$\begin{aligned}
&\sup_{P:W(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] - \sup_{P:W_*(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] \\
&= \inf_{\lambda\ge 0}\{\lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_\lambda^c(Z)]\} - \lambda_*\varepsilon - \mathbb{E}_{Z\sim P_n}[\ell_{\lambda_*}^{c_*}(Z)] \\
&\le \lambda_*\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_{\lambda_*}^c(Z)] - \lambda_*\varepsilon - \mathbb{E}_{Z\sim P_n}[\ell_{\lambda_*}^{c_*}(Z)] \\
&= \mathbb{E}_{Z\sim P_n}[\ell_{\lambda_*}^c(Z) - \ell_{\lambda_*}^{c_*}(Z)].
\end{aligned}$$

By Assumption A3, we have

$$\begin{aligned}
\ell_{\lambda_*}^c(z) - \ell_{\lambda_*}^{c_*}(z) &= \sup_{x_2\in\mathcal{X}}\{\ell(x_2,y) - \lambda_* c((x,y),(x_2,y))\} - \sup_{x_2\in\mathcal{X}}\{\ell(x_2,y) - \lambda_* c_*((x,y),(x_2,y))\} \\
&\le \lambda_* \sup_{x_2\in\mathcal{X}} |c((x,y),(x_2,y)) - c_*((x,y),(x_2,y))| \\
&\le \lambda_*\eta D^2.
\end{aligned}$$

Thus, we conclude that

$$\sup_{P:W(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] - \sup_{P:W_*(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] \le \lambda_*\eta D^2.$$

Similarly, we have

$$\sup_{P:W_*(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] - \sup_{P:W(P,P_n)\le\varepsilon} \mathbb{E}_{Z\sim P}[\ell(Z)] \le \lambda_\dagger\eta D^2,$$

where $\lambda_\dagger \in \arg\min_{\lambda\ge 0}\{\lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_\lambda^c(Z)]\}$.

Now, it suffices to show that $\lambda_* \le \frac{L}{\sqrt{\varepsilon}}$ (and similarly $\lambda_\dagger \le \frac{L}{\sqrt{\varepsilon}}$). By the optimality of λ_*,

$$\begin{aligned}
\lambda_*\varepsilon &\le \lambda_*\varepsilon + \mathbb{E}_{Z\sim P_n}[\sup_{x_2\in\mathcal{X}}\{\ell(x_2,Y) - \lambda_* d_{x_*}^2(X,x_2)\} - \ell(X,Y)] \\
&= \lambda_*\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_{\lambda_*}^{c_*}(Z) - \ell(Z)] \\
&\le \lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\ell_\lambda^{c_*}(Z) - \ell(Z)] \\
&= \lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\sup_{x_2\in\mathcal{X}}\{\ell(x_2,Y) - \ell(X,Y) - \lambda d_{x_*}^2(X,x_2)\}]
\end{aligned}$$

for any $\lambda \geq 0$. By Assumption A2, the right-hand side is at most

$$\begin{aligned}\lambda_* \varepsilon &\leq \lambda\varepsilon + \mathbb{E}_{Z\sim P_n}[\sup_{x_2\in\mathcal{X}}\{Ld_{x_*}(X, x_2) - \lambda d_{x_*}^2(X, x_2)\}] \\ &\leq \lambda\varepsilon + \sup_{t\geq 0}\{Lt - \lambda t^2\}.\end{aligned}$$

We minimize the right-hand side with respect to t (set $t = \frac{L}{2\lambda}$) and λ (set $\lambda = \frac{L}{2\sqrt{\varepsilon}}$) to obtain $\lambda_*\varepsilon \leq L\sqrt{\varepsilon}$, or equivalently $\lambda_* \leq \frac{L}{\sqrt{\varepsilon}}$. □

A.2 Proofs of Theorems in Section 3

Proof of Theorem 3.1. We are working with Euclidean space $\mathbb{D} = \mathbb{R}^K$ and $\mathbb{E} = \mathbb{R}$.

By Theorem 3.4, $\psi : \mathbb{R}^K \to \mathbb{R}$ is Hadamard directionally differentiable at $f_\star$ (tangentially to $\mathbb{R}^K$).

Since f_n is the empirical version of $f_\star$, by central limit theorem, we have

$$\sqrt{n}(f_n - f_\star) \xrightarrow{d} \mathcal{N}(0, \Sigma(f_\star)) \overset{d}{\sim} Z,$$

which is tight and supported in $\mathbb{R}^K$.

Via delta method (Theorem 3.3) with $\psi(\cdot)$ and the derivative formula given by Theorem 3.4, we conclude

$$\sqrt{n}\{\psi(f_n) - \psi(f_\star)\} \xrightarrow{d} \psi'_{f_\star}(Z) = \inf\{(\lambda + l)^\top Z : (\nu, \mu, \lambda) \in \Lambda\}.$$

Hence we complete the proof of Theorem 3.1. □

The next theorem adapted from from Bonnans and Shapiro (2000) will turn out to be useful.

Theorem A.1 (Proposition 4.27 in Bonnans and Shapiro (2000))**.** *$\mathbb{A}$, $\mathbb{B}$ and $\mathbb{V}$ are Banach spaces. $f : \mathbb{A} \to \mathbb{R}$ is continuously differentiable. $G + \bullet : \mathbb{A} \times \mathbb{V} \to \mathbb{B}$ is continuously differentiable. $\mathbb{K}$ is a closed convex subset of $\mathbb{B}$. Consider a class of problems*

$$(\mathcal{P}_v): \quad \min_{x\in\mathbb{A}} \quad f(x) \qquad \text{subject to} \quad G(x) + v \in \mathbb{K}$$

parameterized by $v \in \mathbb{V}$. Let $\varphi(v)$ be the optimal value of the problem $\mathcal{P}_v$. Suppose that

1. *for $v = 0$, the problem $\mathcal{P}_0$ is convex;*
2. *$\varphi(0)$ is finite;*
3. *$0 \in \text{int}\{G(\mathbb{A}) - \mathbb{K}\}$.*

Then the optimal value function $\varphi(v)$ is Hadamard directionally differentiable at $v = 0$. Furthermore,

$$\lim_{h'\to h, t\to 0^+} \frac{\varphi(th') - \varphi(0)}{t} = \sup\{\lambda^\top h : \lambda \in \Gamma\}$$

for any $h \in \mathbb{V}$, where Γ is the set of optimal solutions of the dual problem of $\mathcal{P}_0$.

Proof of Theorem 3.4. We first prove the theorem without constraint $\langle D, \Pi\rangle = 0$. In order to employ Theorem A.1, the result of canonical perturbation, we introduce a parameter $t \in \mathbb{R}$, and the optimization problem $\psi(f_\star)$ can be equivalently rewritten as

$$\begin{aligned}(\text{P1}): \quad &\max_{t\in\mathbb{R}, \Pi\in\mathbb{R}_+^{K\times K}} && l^\top(\Pi^\top \mathbf{1}_K - f_\star) + t \\ &\text{subject to} && \langle C, \Pi\rangle \leq \varepsilon && : \nu \\ &&& \Pi\mathbf{1}_K = f_\star && : \lambda \\ &&& t = 0 && : \eta\end{aligned}$$

where ν, λ, η are Lagrange multipliers.

The canonical perturbation of problem (P1) is then given by

$$(\mathcal{P}_{u,v,w}): \quad \max_{t\in\mathbb{R},\Pi\in\mathbb{R}_+^{K\times K}} \quad l^\top(\Pi^\top \mathbf{1}_K - f_\star) + t$$
$$\text{subject to} \quad \langle C, \Pi\rangle + u \le \varepsilon$$
$$\Pi \mathbf{1}_K + v = f_\star$$
$$t + w = 0,$$

which outputs its optimal value $\varphi(u, v, w)$. Thus φ is a function from $\mathbb{R}^{K+2}$ to $\mathbb{R}$.

Let $\mathbb{A} = \mathbb{R}_+^{K\times K} \times \mathbb{R}$, $\mathbb{B} = \mathbb{V} = \mathbb{R}^{K+2}$, and $\mathbb{K} = \{(x, f_\star^\top, 0)^\top : x \le \varepsilon\} \subset \mathbb{R}^{K+2}$. Consider function $f : \mathbb{A} \to \mathbb{R}$ such that $(\Pi, t) \mapsto -\{l^\top(\Pi^\top \mathbf{1}_K - f_\star) + t\}$, and function $G : \mathbb{A} \to \mathbb{B}$ such that $(\Pi, t) \mapsto (\langle C, \Pi\rangle, (\Pi\mathbf{1}_K)^\top, t)^\top$.

Then, the class of maximization problems $(\mathcal{P}_{u,v,w})$ is equivalent to the following class of minimization problems

$$(\mathcal{Q}_{u,v,w}): \quad \min_{(\Pi,t)\in\mathbb{A}} \quad f(\Pi, t)$$
$$\text{subject to} \quad G(\Pi, t) + (u, v^\top, w)^\top \in \mathbb{K}.$$

Denote the optimal value function of $\mathcal{Q}_{u,v,w}$ by $\phi(u, v, w)$.

(i) To check item 1 in Theorem A.1, we note that $\mathcal{Q}_{0,\mathbf{0}_K,0}$ is a problem of linear programming, and thus a convex optimization problem.

(ii) Item 2 in Theorem A.1 is guaranteed by

$$\varepsilon \ge 0 = \min\{\langle C, \Pi\rangle : \Pi \in \mathbb{R}_+^{K\times K}, \Pi\mathbf{1}_K = f_\star\},$$

which implies that $\mathcal{Q}_{0,\mathbf{0}_K,0}$ has a solution, and thus $\phi(0, \mathbf{0}_K, 0)$ is finite.

(iii) $f_\star \in \mathbb{R}_+^K$ ensures that item 3 in Theorem A.1 holds.

Now applying Theorem A.1 to $(\mathcal{Q}_{u,v,w})$, we conclude that ϕ is Hadamard directionally differentiable at the origin. Note that $\varphi = -\phi$, we can further conclude that φ is also Hadamard directionally differentiable at the origin, and

$$\lim_{\substack{\xi'\to\xi \\ t\to 0^+}} \frac{\varphi(0, t\xi') - \varphi(0, \mathbf{0}_{K+1})}{t} = -\lim_{\substack{\xi'\to\xi \\ t\to 0^+}} \frac{\phi(0, t\xi') - \phi(0, \mathbf{0}_{K+1})}{t} = -\sup\{\langle(\lambda^\top, w)^\top, \xi\rangle : (\nu, \lambda, w) \in \Gamma\},$$

where Γ is the set of optimal solutions of the dual problem of (P1).

Furthermore, one can check that $\Gamma = \Lambda \times \{-1\}$, where Λ is the set of optimal solutions of the dual problem of $\psi(f_\star)$.

Specifically, the dual problem of $\psi(f_\star)$ is given by

$$\min_{\nu\ge 0,\lambda_1,\cdots,\lambda_K} \quad -\varepsilon\nu - \sum_{k=1}^{K} f_\star^{(k)}\lambda_k$$
$$\text{subject to} \quad c_{ij}\nu + \lambda_i \le -l_j, \quad \text{for } 1 \le i, j \le K.$$

Thus, we have

$$\Lambda = \operatorname*{arg\,max}_{\nu,\ge 0,\lambda\in\mathbb{R}^K} \{\varepsilon\nu + f_\star^\top \lambda : c_{ij}\nu + \lambda_i \le -l_j, 1 \le i, j \le K\}$$

Note that $\psi(f) = \varphi(0, f_\star - f, l^\top(f - f_\star))$, we conclude that $\psi(f)$ is Hadamard directionally differentiable at $f_\star$, and the derivative formula is given by

$$\begin{aligned}
\psi'_{f_\star}(h) &= \lim_{\substack{h'\to h\\ t\to 0^+}} \frac{\psi(f_\star + th') - \psi(f_\star)}{t} \\
&= \lim_{\substack{h'\to h\\ t\to 0^+}} \frac{\varphi(0, -th', tl^\top h') - \varphi(0, \mathbf{0}_K, 0)}{t} \\
&= \lim_{\substack{\xi'\to \xi\\ t\to 0^+}} \frac{\varphi(0, t\xi') - \varphi(0, \mathbf{0}_{K+1})}{t} \qquad \left[\text{where } \xi = (-h^\top, l^\top h)^\top\right] \\
&= -\sup\{\langle(\lambda^\top, w)^\top, \xi\rangle : (\nu, \lambda, w) \in \Gamma\} \\
&= -\sup\{\langle(\lambda^\top, -1)^\top, (-h^\top, l^\top h)^\top\rangle : (\nu, \lambda) \in \Lambda\} \\
&= -\sup\{-\langle \lambda + l, h\rangle : (\nu, \lambda) \in \Lambda\} \\
&= \inf\{\langle \lambda + l, h\rangle : (\nu, \lambda) \in \Lambda\}.
\end{aligned}$$

For the case with constraint $\langle D, \Pi\rangle = 0$, note that the dual problem of $\psi(f_\star)$ changes slightly into

$$\begin{aligned}
\min_{\nu,\mu\geq 0,\lambda_1,\cdots,\lambda_K} \quad & -\varepsilon\nu - \sum_{k=1}^{K} f_\star^{(k)}\lambda_k \\
\text{subject to} \quad & c_{ij}\nu + d_{ij}\mu + \lambda_i \leq -l_j, \quad \text{for } 1 \leq i, j \leq K,
\end{aligned}$$

and

$$\Lambda = \operatorname*{arg\,max}_{\nu,\mu\geq 0,\lambda\in\mathbb{R}^K} \{\varepsilon\nu + f_\star^\top\lambda : c_{ij}\nu + d_{ij}\mu + \lambda_i \leq -l_j, 1 \leq i, j \leq K\}.$$

Hence we complete the proof of Theorem 3.4. □

A.3 Proofs of Theorems in Section 4

The following lemma adapted from Hong and Li (2018) provides a general recipe for the consistency of our two bootstrap strategies.

Lemma A.2 (Theorem 3.1 in Hong and Li (2018))**.** *Suppose $\mathbb{D}$ and $\mathbb{E}$ are Banach Spaces and $\phi : \mathbb{D}_\phi \subseteq \mathbb{D} \mapsto \mathbb{E}$ is Hadamard directionally differentiable at θ_0 tangentially to $\mathbb{D}_0$. Let $\hat{\theta}_n : \{X_i\}_{i=1}^n \mapsto \mathbb{D}_\phi$ be such that for some $r_n \uparrow \infty, r_n \left\{\hat{\theta}_n - \theta_0\right\} \rightsquigarrow \mathbb{G}_0$ in $\mathbb{D}$, where $\mathbb{G}_0$ is tight and its support is included in $\mathbb{D}_0$. Then*

$$r_n\left(\phi\left(\hat{\theta}_n\right) - \phi\left(\theta_0\right)\right) \rightsquigarrow \phi'_{\theta_0}\left(\mathbb{G}_0\right).$$

Let $\mathbb{Z}_n^* \rightsquigarrow \mathbb{G}_0$ satisfy regularity of measurability [1]*. Then for $\epsilon_n \to 0, r_n\epsilon_n \to \infty$,*

$$\hat{\phi}'_n\left(\mathbb{Z}_n^*\right) \stackrel{\text{def}}{=\!=} \frac{\phi\left(\hat{\theta}_n + \epsilon_n\mathbb{Z}_n^*\right) - \phi\left(\hat{\theta}_n\right)}{\epsilon_n} \rightsquigarrow \phi'_{\theta_0}\left(\mathbb{G}_0\right).$$

Proof of Theorem 4.1. Hereafter, $\mathbb{G}_0$ refers to $\mathcal{N}(f_\star, \Sigma(f_\star))$. By central limit theorem, we have

$$\sqrt{n}\{f_n - f_\star\} \rightsquigarrow \mathbb{G}_0 \quad \text{and} \quad \sqrt{m}\{f_{n,m}^* - f_\star\} \rightsquigarrow \mathbb{G}_0.$$

Since $m/n \to 0$, we have

$$\sqrt{m}\{f_{n,m}^* - f_n\} = \sqrt{m}\{f_{n,m}^* - f_\star\} - \sqrt{\frac{m}{n}}\sqrt{n}\{f_n - f_\star\} \rightsquigarrow \mathbb{G}_0.$$

[1] $\mathbb{Z}_n^*$ is asymptotically measurable jointly in the data and the bootstrap weights; $g\left(\mathbb{Z}_n^*\right)$ is a measurable function of the bootstrap weights outer almost surely in the data for every bounded, continuous map $g : \mathbb{D} \to \mathbb{R}$; $\mathbb{G}_0$ is Borel measurable and separable.

Let $r_n = \sqrt{n}, \epsilon_n = 1/\sqrt{m}$ and $\mathbb{Z}_n^\star = \sqrt{m}\{f_{n,m}^* - f_n\}$. Then $\epsilon_n \to 0, r_n\epsilon_n \to \infty$, and $\mathbb{Z}_n^\star \rightsquigarrow \mathbb{G}_0$. Applying Lemma A.2, we conclude

$$\begin{aligned}\sqrt{m}\left\{\psi(f_{n,m}^*) - \psi(f_n)\right\} &= \frac{\psi\left(f_n + \frac{1}{\sqrt{m}}\sqrt{m}\{f_{n,m}^* - f_n\}\right) - \psi(f_n)}{1/\sqrt{m}} \\ &= \frac{\psi(f_n + \epsilon_n \mathbb{Z}_n^*) - \psi(f_n)}{\epsilon_n} \rightsquigarrow \psi'_{f_\star}(\mathbb{G}_0).\end{aligned}$$

Finally, note that $\sqrt{n}\{\psi(f_n) - \psi(f_\star)\} \rightsquigarrow \psi'_{f_\star}(\mathbb{G}_0)$, we have

$$\begin{aligned}&\sup_{g\in \mathrm{BL}_1(\mathbb{R})} \left|\mathbb{E}\left[g\left(\sqrt{m}\left\{\psi(f_{n,m}^*) - \psi(f_n)\right\}\right)|f_n\right] - \mathbb{E}\left[g\left(\sqrt{n}\left\{\psi(f_n) - \psi(f_\star)\right\}\right)\right]\right| \\ \le &\sup_{g\in \mathrm{BL}_1(\mathbb{R})} \left|\mathbb{E}\left[g\left(\sqrt{m}\left\{\psi(f_{n,m}^*) - \psi(f_n)\right\}\right)|f_n\right] - \mathbb{E}\left[g\left(\psi'_{f_\star}(\mathbb{G}_0)\right)\right]\right| \\ &+ \sup_{g\in \mathrm{BL}_1(\mathbb{R})} \left|\mathbb{E}\left[g\left(\psi'_{f_\star}(\mathbb{G}_0)\right)\right] - \mathbb{E}\left[g\left(\sqrt{n}\left\{\psi(f_n) - \psi(f_\star)\right\}\right)\right]\right| \\ &= o_p(1) + o_p(1) = o_p(1)\end{aligned}$$

by triangle inequality. Hence we complete the proof of Theorem 4.1. □

Proof of Theorem 4.2. By central limit theorem, we have

$$\sqrt{n}\{f_n - f_\star\} \rightsquigarrow \mathbb{G}_0 \sim \mathcal{N}(\mathbf{0}_k, \Sigma(f_\star)).$$

As $\epsilon \to 0, n \to \infty$, we have

$$\mathbb{T}(f_n, \epsilon) \to \mathbb{R}^K \quad \text{and} \quad z_n^* \sim \mathcal{N}(\mathbf{0}_K, \Sigma(f_n); \mathbb{T}) \rightsquigarrow \mathcal{N}(\mathbf{0}_k, \Sigma(f_\star)) \sim \mathbb{G}_0.$$

Let $r_n = \sqrt{n}, \epsilon_n = \epsilon$, and $\mathbb{Z}_n^* = z_n^*$. Then $\epsilon_n \to 0, r_n\epsilon_n \to \infty$, and $\mathbb{Z}_n^\star \rightsquigarrow \mathbb{G}_0$. Applying Lemma A.2, we conclude

$$\epsilon^{-1}\left\{\psi(f_n + \epsilon z_n^*) - \psi(f_n)\right\} = \frac{\psi(f_n + \epsilon_n \mathbb{Z}_n^*) - \psi(f_n)}{\epsilon_n} \rightsquigarrow \psi'_{f_\star}(\mathbb{G}_0).$$

Similar to the previous proof, note that $\sqrt{n}\{\psi(f_n) - \psi(f_\star)\} \rightsquigarrow \psi'_{f_\star}(\mathbb{G}_0)$, we have

$$\begin{aligned}&\sup_{g\in \mathrm{BL}_1(\mathbb{R})} \left|\mathbb{E}\left[g\left(\epsilon^{-1}\left\{\psi(f_n + \epsilon z_n^*) - \psi(f_n)\right\}\right)|f_n\right] - \mathbb{E}\left[g\left(\sqrt{n}\left\{\psi(f_n) - \psi(f_\star)\right\}\right)\right]\right| \\ \le &\sup_{g\in \mathrm{BL}_1(\mathbb{R})} \left|\mathbb{E}\left[g\left(\epsilon^{-1}\left\{\psi(f_n + \epsilon z_n^*) - \psi(f_n)\right\}\right)|f_n\right] - \mathbb{E}\left[g\left(\psi'_{f_\star}(\mathbb{G}_0)\right)\right]\right| \\ &+ \sup_{g\in \mathrm{BL}_1(\mathbb{R})} \left|\mathbb{E}\left[g\left(\psi'_{f_\star}(\mathbb{G}_0)\right)\right] - \mathbb{E}\left[g\left(\sqrt{n}\left\{\psi(f_n) - \psi(f_\star)\right\}\right)\right]\right| \\ &= o_p(1) + o_p(1) = o_p(1)\end{aligned}$$

by triangle inequality. Hence we complete the proof of Theorem 4.2. □

Proof of Theorem 4.3. By standard results in Politis et al. (1999), under bootstrap consistency, we have

$$\liminf_{n\to\infty} \mathbb{P}\left(\psi(f_\star) \in \left[\psi(f_n) - \frac{c_{1-\alpha/2}^*}{\sqrt{n}}, \psi(f_n) - \frac{c_{\alpha/2}^*}{\sqrt{n}}\right]\right) = 1 - \alpha$$

if the limiting distribution is continuous at the boundary of quantiles;

$$\liminf_{n\to\infty} \mathbb{P}\left(\psi(f_\star) \in \left[\psi(f_n) - \frac{c_{1-\alpha/2}^*}{\sqrt{n}}, \psi(f_n) - \frac{c_{\alpha/2}^*}{\sqrt{n}}\right]\right) > 1 - \alpha$$

if the limiting distribution is discontinuous at the boundary of quantiles. □

Proof of Theorem 4.5. For any $f_\star \in \Delta_K$ such that $\psi(f_\star) \le \delta$,

$$\begin{aligned}
&\mathbb{P}\left(\sqrt{n}\psi(f_n) > \sqrt{n}\delta + c_{1-\alpha}\right) \\
=&1 - \mathbb{P}\left(\sqrt{n}\psi(f_n) \le \sqrt{n}\delta + c_{1-\alpha}\right) \\
=&1 - \mathbb{P}\left(\sqrt{n}\{\psi(f_n) - \psi(f_\star)\} \le c_{1-\alpha} + \sqrt{n}(\delta - \psi(f_\star))\right) \\
\le&1 - \mathbb{P}(\sqrt{n}\{\psi(f_n) - \psi(f_\star)\} \le c_{1-\alpha}) \\
\le&1 - (1-\alpha) \\
=&\alpha,
\end{aligned}$$

where $c_{1-\alpha}$ is the $(1-\alpha)$-th quantile of $\sqrt{n}\{\psi(f_n) - \psi(f_\star)\}$. With Bootstrap consistency,

$$\begin{aligned}
&\limsup_{n\to\infty} \sup_{f_\star\in\Delta_K:\psi(f_\star)\le\delta} \mathbb{P}_{f_\star}\left(\sqrt{n}\psi(f_n) > \sqrt{n}\delta + c^*_{1-\alpha}\right) \\
\le&\limsup_{n\to\infty} \sup_{f_\star\in\Delta_K:\psi(f_\star)\le\delta} \mathbb{P}_{f_\star}\left(\sqrt{n}\psi(f_n) > \sqrt{n}\delta + c_{1-\alpha}\right) = \alpha.
\end{aligned}$$

For any $f_\star \in \Delta_K$ such that $\psi(f_\star) > \delta$,

$$\mathbb{P}\left(\sqrt{n}\psi(f_n) > \sqrt{n}\delta + c^*_{1-\alpha}\right) \to 1.$$

□

B Bootstrap methods

Algorithm 1 m-out-of-n bootstrap

require: m (rule of thumb: $2\sqrt{n}$), $B \in \mathbb{N}$
set $\mathcal{S} = \varnothing$
for $i = 1, 2, \cdots, B$ **do**:
  draw $Y^* \sim \text{Multinomial}(m; f_n)$
  append $\sqrt{m}\{\psi(Y^*/m) - \psi(f_n))\}$ to $\mathcal{S}$
end for
output: $\mathcal{S}$

Algorithm 2 numerical derivative method

require: ϵ (rule of thumb: $n^{-1/4}$), $B \in \mathbb{N}$
set $\mathcal{S} = \varnothing$, $i = 1$
while $i \le B$ **do**:
  draw $Z^* \sim \mathcal{N}(\mathbf{0}_K, \Sigma(f_n))$
  if $f_n + \epsilon Z^* \in \mathbb{R}^K_+$:
    append $\epsilon^{-1}\{\psi(f_n + \epsilon Z^*) - \psi(f_n))\}$ to $\mathcal{S}$
    $i \leftarrow i + 1$
  else:
    continue
output: $\mathcal{S}$