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the multistep-multiscale bootstrap resampling

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RUNNING HEAD: DETAILS OF MULTISCALE BOOTSTRAP

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Supplement Material to “Approximately unbiased tests of regions using multistep-multiscale bootstrap resampling.”

Summary

The technical details of the new bootstrap method of Shimodaira (2004) are given here in mathematical proofs as well as a supporting computer program. Approximately unbiased tests based on the bootstrap probabilities are considered in Shimodaira (2004) for the exponential family of distributions with unknown expectation parameter vector, where the null hypothesis is represented as an arbitrary-shaped region with smooth boundaries. It has been described in the lemmas of Shimodaira (2004) that the newly developed three-step multiscale bootstrap method calculates an asymptotically third-order accurate p -value. All the mathematical proofs of these lemmas are shown here. The straightforward, though very tedious, calculations involving tensor notations are verified in Shimodaira (2003), which is, in fact, a computer program for *Mathematica*. Here we also give a brief explanation of this program.

A Mathematical proofs of lemmas.

The proofs of Lemma 1 to Lemma 7 of Shimodaira (2004) are presented here. The equation numbers indicate those of Shimodaira (2004) except for those defined here.

A.1 Proof of Lemma 1.

The expression of $f(y; \eta)$ is obtained from (7.1) using the Taylor series of the reparameterization $\theta^i \approx \eta_i + \frac{1}{2}\phi^{ijk}\eta_j\eta_k + \frac{1}{6}\phi^{ijkl}\eta_j\eta_k\eta_l$. The expressions for $\psi(\theta)$ and $h(y)$ are shown in Shimodaira (2003);

$$(A.1) \quad \psi(\theta) \approx \psi(0) + \frac{1}{2}(\eta_i)^2 + \frac{1}{3}\phi^{ijk}\eta_i\eta_j\eta_k + \frac{1}{8}\phi^{ijkl}\eta_i\eta_j\eta_k\eta_l,$$

$$(A.2) \quad h(y) \approx -\psi(0) + \frac{1}{2}p \log(2\pi) + \frac{1}{8}\phi^{iijj} - \frac{1}{6}(\phi^{ijk})^2 - \frac{1}{2}\phi^{iijj}y_i \\ + \frac{1}{2}(\delta_{ij} + \frac{1}{2}\phi^{ikl}\phi^{jkl} - \frac{1}{2}\phi^{ijkk})y_iy_j + \frac{1}{6}\phi^{ijk}y_iy_jy_k + \frac{1}{24}\phi^{ijkl}y_iy_jy_ky_l.$$

By substituting (A.1) and (A.2) for those in (7.1), $f(y; \eta)$ is expressed by y , η , and the derivatives of $\phi(\eta)$ at $\eta = 0$. Then, (7.4) is obtained from $f(\hat{u}, \hat{v}; \lambda) = f(\eta(\hat{u}, \hat{v}); (0, \dots, 0, \lambda))J(\hat{u}, \hat{v})$, where $J(\hat{u}, \hat{v})$ is the Jacobian shown below.

The following lemma gives the Jacobian for the change of variables, which is analogous to that for the tube formula of Weyl (1939). The proof is due to Satoshi Kuriki (pers. comm.); see Lemma 2.1 of Kuriki and Takemura (2000) for the normal case.

Lemma 8 *The Jacobian $J(u, v) = \partial\eta/\partial(u, v)$ is expressed as*

$$\begin{aligned}
& \log J(u, v) \\
& \approx -\frac{1}{2}\phi^{cpp}u_c + (2d^{aa} - \phi^{aap})v - \left\{2(d^{ab})^2 - 2d^{ab}\phi^{abp} + \frac{1}{2}(\phi^{abp})^2\right\}v^2 \\
& + \left\{\frac{1}{2}d^{cd}\phi^{ppp} - \frac{1}{4}\phi^{cdpp} + \frac{1}{4}\phi^{cpp}\phi^{dpp} + \frac{1}{2}\phi^{acp}\phi^{adp} + 2d^{ac}(d^{ad} - \phi^{adp})\right\}u_cu_d \\
& + \left\{6e^{aac} + d^{aa}\phi^{cpp} + 4d^{ac}\phi^{app} - \phi^{aacp} + \phi^{aad}\phi^{cdp} \right. \\
& \quad \left. + \frac{1}{2}\phi^{aap}\phi^{cpp} - 2d^{cd}\phi^{aad} - (2d^{ad} - \phi^{adp})\phi^{acd}\right\}u_cv.
\end{aligned}$$

Proof. Considering the projection of $d\eta_i = B_i^a(u)du_a + B_i^p(u)dv + v(\partial B_i^p/\partial u_a)du_a$ to the tangent vectors and the normal vector, we get

$$(A.3) \quad \begin{pmatrix} B_i^a(u) \\ B_i^p(u) \end{pmatrix} \phi^{ij}(\eta(u))d\eta_j \approx \begin{pmatrix} \phi^{ac}(u) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \delta_{cb} + vc_c^b(u) & 0 \\ vc_p^b(u) & 1 \end{pmatrix} \begin{pmatrix} du_b \\ dv \end{pmatrix},$$

where $c_b^a(u)$ and $c_p^a(u)$ are defined by $(\partial B_i^p/\partial u_a) = c_b^a(u)B_i^b(u) + c_p^a(u)B_i^p(u)$. We have used a simplified notation in which $\phi^{ac}(u)$, say, in the partitioned matrix implies the $(p-1) \times (p-1)$ matrix instead of the (a, c) -element of the matrix. It follows from the definition of the metric that the determinant of the $p \times p$ matrix on the left hand side of (A.3) is

$$\det \left\{ \begin{pmatrix} B_i^a(u) \\ B_i^p(u) \end{pmatrix} \phi^{ij}(\eta(u)) \right\} = \left\{ \det(\phi^{ab}(u)) \det(\phi^{ij}(\eta(u))) \right\}^{\frac{1}{2}}.$$

Hence we find from (A.3) that the logarithm of the Jacobian is expressed as $\log J(u, v) = \frac{1}{2} \log \det(\phi^{ab}(u)) + \log \det(\delta_{ab} + vc_c^b(u)) - \frac{1}{2} \log \det(\phi^{ij}(\eta(u)))$. Using the inverse matrix of $\phi^{ab}(u)$ with components $\phi_{ab}(u) \approx \delta_{ab} - \phi^{abc}u_c - \{4d^{ac}d^{bd} - 2d^{ac}\phi^{bdp} - 2d^{bd}\phi^{acp} - d^{cd}\phi^{abp} - \phi^{ace}\phi^{bde} + \frac{1}{2}\phi^{abcd}\}u_cu_d$, the elements of $c_b^a(u)$ is given by $c_b^a(u) = (\partial B_i^p/\partial u_a)\phi^{ij}(\eta(u))B_j^c(u)\phi_{cb}(u)$, and therefore the proof completes by noting the formal expansions $\log \det(I_p + A) = \text{tr}(A) - \frac{1}{2}\text{tr}(A^2) + \frac{1}{3}\text{tr}(A^3) + \dots$, and $(I_p + A)^{-1} = I_p - A + A^2 - A^3 + \dots$ for $p \times p$ matrix A .

A.2 Proof of Lemma 2.

Let the density function of X be $\exp(\theta_X^i x_i - \psi_X(\theta_X) - h_X(x))$, where $\theta_X = (\theta_X^1, \dots, \theta_X^p)$ is the natural parameter and $\mu = \partial\psi_X/\partial\theta_X$ is the expectation parameter. The cumulant function of the simple sum $S = X_1 + \dots + X_m$ is $m\psi_X(\theta_X)$ and the expectation parameter is $\eta_S = m\mu$. The potential function of S is then $\phi_S(\eta_S) = \max_{\theta_X} \{\theta_X' \eta_S - m\psi_X(\theta_X)\} = m\phi_X(\eta_S/m)$. Since $Y = (\sqrt{n}/m)S$ has the same potential as S , we obtain the potential of Y as $\phi_Y(\eta) = m\phi_X(\eta/\sqrt{n})$ with expectation $\eta = (\sqrt{n}/m)\eta_S = \sqrt{n}\mu$. For $m = n$, it follows from the assumption that $n\phi_X(\eta/\sqrt{n}) = \phi(\eta)$. This implies $\phi_Y(\eta) = (m/n)\phi(\eta) = \phi(\eta)/\tau^2$ for $m > 0$.

A.3 Proof of Lemma 3.

We work on a random vector $\tilde{Y} = Y/\tau$, to which the argument of the previous section is easily applied. The potential function is $\tilde{\phi}(\tilde{\eta}, \tau) = \phi(\eta, \tau)$ with expectation parameter $\tilde{\eta} = \eta/\tau$. Noting the k -th derivative is $\partial^k \tilde{\phi}(\tilde{\eta}, \tau)/\partial \tilde{\eta}^k = \tau^{k-2} \partial^k \phi(\eta, 1)/\partial \eta^k$, and especially the metric $\partial^2 \tilde{\phi}(\tilde{\eta}, \tau)/\partial \tilde{\eta}_i \partial \tilde{\eta}_j = \partial^2 \phi(\eta)/\partial \eta_i \partial \eta_j$ is δ_{ij} at $\tilde{\eta} = 0$, Lemma 1 is applied immediately to \tilde{Y} by the replacement (7.7). The tube-coordinates (u, v) is replaced by $(\tilde{u}, \tilde{v}) \leftrightarrow \tilde{\eta}$, which should be given by going back to the specification of $\eta(u)$ and $B^p(u)$ using $\tilde{\phi}(\tilde{\eta}, \tau)$ instead of $\phi(\eta, 1)$. Fortunately a simple transformation (7.6) is consistent with the specification, and thus the joint density of (\tilde{u}, \tilde{v}) is easily brought back to that of (u, v) . The expression of $\log f(u, v; \lambda, \tau)$, although not shown to save the space, is then obtained from (7.4) by these replacements, and by adding the logarithm of the Jacobian to it.

A.4 Proof of Lemma 4.

We first consider the case $\tau = 1$ to derive the cumulants $\kappa_1, \kappa_2, \dots$, of \hat{w} . The joint density of (\hat{u}, \hat{w}) is $f(u, w; \lambda) = f(u, v(u, w); \lambda)(\partial v/\partial w)$, where the Jacobian is $\partial v/\partial w = \exp\{-\sum_{r \geq 1} (c_r + u_c b_r^c) r w^{r-1} - \frac{1}{2}(\sum_{r \geq 1} c_r r w^{r-1})^2\}$. By rearranging the formula, $f(u, w; \lambda)$ is expressed in the form

$$(A.4) \quad (2\pi)^{-\frac{p-1}{2}} \exp\left(-\frac{1}{2}u_a u_a\right) \\ \times \exp\left(A + A^a u_a + A^{ab} u_a u_b + A^{abc} u_a u_b u_c + A^{abcd} u_a u_b u_c u_d\right) + O(n^{-3/2}),$$

where the coefficients $A = O(1)$, $A^a = O(n^{-1/2})$, $A^{ab} = O(n^{-1/2})$, $A^{abc} = O(n^{-1/2})$, and $A^{abcd} = O(n^{-1})$ are functions of w and λ . We obtain the marginal density of w by integrating (A.4) with respect to u . The logarithm of it is $A + A^{aa} + 3A^{aabb} + \frac{1}{2}A^a A^a + A^{ab} A^{ab} + 3A^a A^{abb} + \frac{9}{2}A^{aac} A^{bbc} + 3A^{abc} A^{abc} + O(n^{-3/2})$, which becomes $\log f(w; \lambda) \approx -\frac{1}{2} \log(2\pi) - \frac{1}{2}(w - \lambda)^2 + \left[(d^{ab})^2 - \frac{1}{2}d^{aa} d^{bb} - d^{ab} \phi^{abp} + \frac{1}{2}(\phi^{abp})^2 + \frac{1}{2}(\phi^{app})^2 + \frac{1}{6}(\phi^{ppp})^2 - \frac{1}{4}\phi^{aapp} - \frac{1}{8}\phi^{pppp} - d^{aa} \lambda + (d^{ab})^2 \lambda^2 - \frac{1}{2}d^{aa} \phi^{ppp} \lambda^2 - \frac{1}{3}\phi^{ppp} \lambda^3 - \frac{1}{8}\phi^{pppp} \lambda^4 + \frac{1}{8}(\phi^{app})^2 \lambda^4 \right] + w \left[d^{aa} + \frac{1}{2}\phi^{ppp} + \left\{ -d^{ab} \phi^{abp} + \frac{1}{2}d^{aa} \phi^{ppp} + \frac{1}{2}(\phi^{abp})^2 + \frac{3}{8}(\phi^{app})^2 - \frac{1}{4}\phi^{aapp} \right\} \lambda + \frac{1}{2}\phi^{ppp} \lambda^2 + \frac{1}{6}\phi^{pppp} \lambda^3 - \frac{1}{4}(\phi^{app})^2 \lambda^3 \right] + w^2 \left[-(d^{ab})^2 + d^{ab} \phi^{abp} - \frac{1}{2}(\phi^{abp})^2 - \frac{1}{2}(\phi^{app})^2 - \frac{1}{4}(\phi^{ppp})^2 + \frac{1}{4}\phi^{pppp} + \frac{1}{4}\phi^{aapp} + \frac{1}{8}(\phi^{app})^2 \lambda^2 \right] - \frac{1}{6}\phi^{ppp} w^3 - \frac{1}{24}\phi^{pppp} w^4 + (\sum_i c_i w^i) \left\{ w - \lambda - d^{aa} - \frac{1}{2}\phi^{ppp} + \frac{1}{2}\phi^{ppp} w^2 - \frac{1}{2}\phi^{ppp} \lambda^2 - \frac{1}{6}\phi^{pppp} \lambda^3 \right\} - \frac{1}{2}(\sum_i c_i w^i)^2 - \sum_i i c_i w^{i-1} - \frac{1}{2}(\sum_i i c_i w^{i-1})^2$. For a parameter t , consider the formal expansion

$$(A.5) \quad e^{wt} f(w; \lambda) \approx (2\pi)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(w - (\lambda + t))^2\right) \\ \times \exp\left(B_0 + B_1 w + B_2 w^2 + B_3 w^3 + B_4 w^4\right),$$

where the coefficients B_r are functions of t and λ . By integrating (A.5) with respect to w , and taking the logarithm of it, we obtain $B_0 + B_2 + 3B_4 + \frac{1}{2}B_1^2 + B_2^2 + 3B_1B_3 + \frac{15}{2}B_3^2 + (\lambda+t)(B_1 + 3B_3 + 2B_1B_2 + 12B_2B_3) + (\lambda+t)^2(B_2 + 6B_4 + 3B_1B_3 + 2B_2^2 + 18B_3^2) + (\lambda+t)^3(B_3 + 6B_2B_3) + (\lambda+t)^4(B_4 + \frac{9}{2}B_3^2)$. This is compared with $\log \int e^{wt} f(w; \lambda) dw = t\kappa_1 + \frac{t^2}{2}\kappa_2 + \frac{t^3}{6}\kappa_3 + \frac{t^4}{24}\kappa_4 + \dots$ to obtain $\kappa_1 \approx d^{aa} + c_0 + c_2 + \left\{ 1 - 2(d^{ab})^2 + d^{ab}\phi^{abp} - \frac{1}{2}d^{aa}\phi^{ppp} - \frac{1}{2}(\phi^{abp})^2 - \frac{5}{8}(\phi^{app})^2 + \frac{1}{4}\phi^{aapp} + c_1 + 2c_0c_2 + c_2(2d^{aa} - \phi^{ppp}) + 3c_3 + 6c_2^2 \right\} \lambda + c_2\lambda^2 + (c_3 + 2c_2^2)\lambda^3$, $\kappa_2 \approx 1 - 2(d^{ab})^2 + 2d^{ab}\phi^{abp} - d^{aa}\phi^{ppp} - (\phi^{abp})^2 - (\phi^{app})^2 + \frac{1}{2}\phi^{aapp} + 2c_1 + 2c_2(2d^{aa} - \phi^{ppp}) + 6c_3 + 4c_0c_2 + 14c_2^2 + (-\phi^{ppp} + 4c_2)\lambda + \left\{ \frac{1}{4}(\phi^{app})^2 + (\phi^{ppp})^2 - \frac{1}{2}\phi^{pppp} - 4c_2\phi^{ppp} + 6c_3 + 16c_2^2 \right\} \lambda^2$, $\kappa_3 \approx -\phi^{ppp} + 6c_2 + \left\{ 3(\phi^{ppp})^2 - \phi^{pppp} - 18c_2\phi^{ppp} + 18c_3 + 60c_2^2 \right\} \lambda$, $\kappa_4 \approx 3(\phi^{ppp})^2 - \phi^{pppp} - 24c_2\phi^{ppp} + 24c_3 + 96c_2^2$, and $\kappa_r \approx 0$ for $r \geq 5$.

The expression of $z_c(\hat{w}; \lambda, 1)$ is obtained by applying the Cornish-Fisher series (Johnson and Kotz, p. 66, 1994) to these cumulants of \hat{w} . The expression of $z_c(\hat{w}; \lambda, \tau)$ is then obtained by the replacements of Lemma 3, and by replacing c_r with $\tilde{c}_r = c_r\tau^{r-1}$.

A.5 Proof of Lemma 5.

Let us consider the local coordinates $\Delta\eta$ at $\eta(\hat{u})$ so that $\eta(\hat{u})$ becomes the origin;

$$\eta_i = \eta_i(\hat{u}) + B_i^j(\hat{u})\Delta\eta_j, \quad i = 1, \dots, p$$

defines the reparameterization $\eta \leftrightarrow \Delta\eta$ at each \hat{u} . The surface is now represented in the $\Delta\eta$ -coordinates as $\Delta\eta_p \approx -\hat{d}^{ab}\Delta\eta_a\Delta\eta_b - \hat{e}^{abc}\Delta\eta_a\Delta\eta_b\Delta\eta_c$ using the Taylor coefficients at $\eta(\hat{u})$; $\hat{d}^{ab} \approx d^{ab} + (\frac{1}{2}d^{ab}\phi^{cpp} + 3e^{abc})\hat{u}_c$ and $\hat{e}^{abc} \approx e^{abc}$. The derivatives $\hat{\phi}^{ij}$, $\hat{\phi}^{ijk}$, and $\hat{\phi}^{ijkl}$ of $\phi(\eta)$ at $\eta(\hat{u})$ with respect to $\Delta\eta$ -coordinates are obtained by comparing both sides of

$$\phi^{kl}(\eta)B_k^i(\hat{u})B_l^j(\hat{u}) = \hat{\phi}^{ij} + \hat{\phi}^{ijk}\Delta\eta_k + \frac{1}{2}\hat{\phi}^{ijkl}\Delta\eta_k\Delta\eta_l + \dots$$

The second derivatives are $\hat{\phi}^{ab} = \phi^{ab}(\hat{u})$ of (7.2), $\hat{\phi}^{ap} = 0$, and $\hat{\phi}^{pp} = 1$. The third derivative to the normal direction, i.e., $\hat{\phi}^{ppp} = -6\hat{u}$, is (7.11). The expressions for the other $\hat{\phi}^{ijk} = \phi^{ijk} + O(n^{-1})$ are shown in Shimodaira (2003). The fourth derivatives are $\hat{\phi}^{ijkl} \approx \phi^{ijkl}$.

Although we assumed that $\phi^{ij} = \delta_{ij}$ at the origin in (7.4), the metric changes to $\hat{\phi}^{ij}$ at $\eta(\hat{u})$. We have to multiply the matrix $(\hat{\phi}^{ij})^{-1/2}$ to the vector $\Delta\eta$ to bring back the metric to the identity matrix. This is equivalent to replacing δ_{ab} in the summation over the indices a, b with $\hat{\phi}_{ab} = \phi_{ab}(\hat{u})$ given in the proof of Lemma 8.

Consequently, $d^{aa} = d^{ab}\delta_{ab}$ in (7.10) is replaced with $\hat{d}^{ab}\hat{\phi}_{ab} = \hat{d}_1$ of (7.12). ϕ^{ppp} in (7.10) is simply replaced with $\hat{\phi}^{ppp}$ of (7.11). $O(n^{-1})$ terms change only $O(n^{-3/2})$; for example, $d_2 = d^{ab}d^{ab} = d^{ab}\delta_{bc}d^{cd}\delta_{da}$ becomes $\hat{d}_2 = \hat{d}^{ab}\hat{\phi}_{bc}\hat{d}^{cd}\hat{\phi}_{da} \approx (d^{ab})^2$.

A.6 Proof of Lemma 6.

$\hat{z}_q(y)$ is expressed as \hat{w} , since \bar{c}_r for $\hat{z}_q(y)$ is that for $\hat{z}_\infty(y)$ plus q_r . Then the coefficients c_r for $\hat{z}_q(y)$ are calculated as $c_0 = -d^{aa} - \frac{1}{6}\phi^{ppp} + q_0$, $c_1 = (d^{ab})^2 - d^{ab}\phi^{abp} + \frac{1}{2}d^{aa}\phi^{ppp} + \frac{1}{2}(\phi^{abp})^2 + \frac{1}{2}(\phi^{app})^2 + \frac{17}{72}(\phi^{ppp})^2 - \frac{1}{4}\phi^{aapp} - \frac{1}{8}\phi^{pppp} + \frac{1}{3}\phi^{ppp}(q_2 - q_0) + q_1 + 2d^{aa}q_2 - 2q_0q_2$, $c_2 = \frac{1}{6}\phi^{ppp} + q_2$, $c_3 = -\frac{5}{72}(\phi^{ppp})^2 + \frac{1}{24}\phi^{pppp} - \frac{2}{3}\phi^{ppp}q_2 - 2q_2^2 + q_3$. By applying Lemma 4 to $z_c(\hat{w}; \lambda, 1)$ with these coefficients, we obtain the distribution function of $\hat{z}_q(y)$.

A.7 Proof of Lemma 7.

We derive the expression of $\tilde{z}_2(\eta(0, \lambda), \tau_1, \tau_2)$ so that $\tilde{z}_2(y, \tau_1, \tau_2)$ is obtained by the replacements of Lemma 5. By letting $y = \eta(0, \lambda)$, the right hand side of (7.18) becomes

$$(A.6) \quad \tilde{z}_2(\eta(0, \lambda), \tau_1, \tau_2) = \Phi^{-1} \left\{ \iint \Phi(\tilde{z}_1(\eta(\hat{u}, \hat{v}), \tau_2)) f(\hat{u}, \hat{v}; \lambda, \tau_1) d\hat{u} d\hat{v} \right\} \\ \approx \Phi^{-1} \left\{ \int \Phi(\tilde{z}_1(\eta(0, \hat{v}), \tau_2)) f(\hat{v}; \lambda, \tau_1) d\hat{v} \right\},$$

where the last approximation follows from the fact that \hat{u} and \hat{v} are approximately independent ignoring $O(n^{-1/2})$ terms; $\log f(\hat{u}, \hat{v}; \lambda, \tau) = -\frac{1}{2}p \log(2\pi\tau) - \frac{1}{2}(\hat{v} - \lambda)^2 \tau^{-2} - \frac{1}{2}(\hat{u}_a)^2 \tau^{-2} + O(n^{-1/2})$, and hence terms of $\bar{b}_r^c = O(n^{-1})$ in (7.8) for $\tau_2 \tilde{z}_1(y, \tau_2)$ contribute only $O(n^{-3/2})$ in the integration.

To carry out the integration of (A.6), we consider a transformation described below. Let us define a generalization of the pivot by $z_\infty(\hat{u}, \hat{v}; \lambda, \tau) := z_c(\hat{v}; \hat{u}, \lambda, \tau)$ with all $c_r = 0$. This reduces to $\hat{z}_\infty(y)$ when $\lambda = 0$ and $\tau = 1$, and a similar argument as Section 7.5 shows that $\Pr\{z_\infty(\hat{U}, \hat{V}; \lambda, \tau) \leq x; \lambda, \tau\} \approx \Phi(x)$. By solving $z_\infty(\hat{u}, v; \lambda, \tau) = z$ for v , we define the inverse function $v_\infty(\hat{u}, z; \lambda, \tau)$, which satisfies $z_\infty(\hat{u}, v_\infty(\hat{u}, z; \lambda, \tau); \lambda, \tau) = z$. Using (7.9), we may obtain $v_\infty(0, z; \lambda, \tau) \approx \lambda + \tau z \left[1 - \frac{1}{2}\phi^{ppp}\lambda + \left(\frac{1}{8}(\phi^{app})^2 + \frac{3}{8}(\phi^{ppp})^2 - \frac{1}{4}\phi^{pppp}\right)\lambda^2 \right] + \tau^2 \left[d^{aa} + \frac{1}{6}\phi^{ppp} + \left(-2(d^{ab})^2 + \frac{1}{4}\phi^{aapp} + d^{ab}\phi^{abp} - \frac{1}{2}(\phi^{abp})^2 - \frac{5}{8}(\phi^{app})^2 - \frac{1}{2}d^{aa}\phi^{ppp} - \frac{1}{3}(\phi^{ppp})^2 + \frac{1}{6}\phi^{pppp}\right)\lambda + z^2 \left(-\frac{1}{6}\phi^{ppp} + \left(\frac{1}{3}(\phi^{ppp})^2 - \frac{1}{6}\phi^{pppp}\right)\lambda\right) \right] + \tau^3 \left[z \left(- (d^{ab})^2 + \frac{1}{4}\phi^{aapp} + d^{ab}\phi^{abp} - \frac{1}{2}(\phi^{abp})^2 - \frac{1}{2}(\phi^{app})^2 - \frac{1}{2}d^{aa}\phi^{ppp} - \frac{17}{72}(\phi^{ppp})^2 + \frac{1}{8}\phi^{pppp}\right) + z^3 \left(\frac{5}{72}(\phi^{ppp})^2 - \frac{1}{24}\phi^{pppp}\right) \right]$.

Considering $\tilde{z}_1(\eta(0, v_\infty(0, z; \lambda, \tau_1)), \tau_2) = (\lambda + z\tau_1)\tau_2^{-1} + O(n^{-1/2})$, and $\Phi(x + \delta) \approx \Phi(x) + f(x)(\delta - \frac{1}{2}x\delta^2)$ for $x = O(1)$ and $\delta = O(n^{-1/2})$, we find that the integration (A.6)

is now expressed as

$$(A.7) \quad \Phi^{-1} \left\{ \int \Phi \left(\tilde{z}_1(\eta(0, v_\infty(0, z; \lambda, \tau_1)), \tau_2) \right) f(z) dz \right\} \\ \approx \Phi^{-1} \left\{ \int \left(\Phi(az + b) + f(az + b) \sum_{r=0}^5 A_r z^r \right) f(z) dz \right\},$$

where $f(z)$ is the standard normal density function, and $a = \tau_1 \tau_2^{-1}$, $b = \lambda \tau_2^{-1}$, and $A_r = O(n^{-1/2})$ are independent of z . The expressions for A_r are not shown here to save the space, but they are functions of the geometric quantities as well as λ , τ_1 , and τ_2 . Let $c = b(1 + a^2)^{-1/2}$. Using $\int_{-\infty}^{\infty} \Phi(az + b) f(z) dz = \Phi(c)$ and $g_r = \int_{-\infty}^{\infty} z^r f(az + b) f(z) dz / f(c)$, the integration (A.7) is expressed as

$$(A.8) \quad \Phi^{-1} \left\{ \Phi(c) + f(c) \sum_{r=0}^5 A_r g_r \right\},$$

where $g_0 = (1 + a^2)^{-1/2}$, $g_1 = -ab(1 + a^2)^{-1} g_0$, $g_2 = (1 + a^2(1 + b^2))(1 + a^2)^{-2} g_0$, $g_3 = -ab(3 + a^2(3 + b^2))(1 + a^2)^{-3} g_0$, $g_4 = (3 + 6a^2(1 + b^2) + a^4(3 + 6b^2 + b^4))(1 + a^2)^{-4} g_0$, and $g_5 = -ab(15 + 10a^2(3 + b^2) + a^4(15 + 10b^2 + b^4))(1 + a^2)^{-5} g_0$. To derive g_r , we may use $\int_{-\infty}^{\infty} z^{2r} f(z) dz = (2r)! / (2^r r!)$, which becomes 1, 3, 15, 105, 945, say, for $r = 1, 2, 3, 4, 5$.

By noting $\Phi^{-1}(\Phi(x) + f(x)\delta) \approx x + \delta + \frac{1}{2}x\delta^2$ for $x = O(1)$ and $\delta = O(n^{-1/2})$, we finally obtain from (A.8) that

$$(A.9) \quad \tilde{z}_2(\eta(0, \lambda), \tau_1, \tau_2) \approx c \left\{ 1 + \frac{1}{2} \left(\sum_{r=0}^5 A_r g_r \right)^2 \right\} + \sum_{r=0}^5 A_r g_r.$$

It is straightforward, though very tedious, to verify that (A.9) is in fact equivalent to $\zeta_3(\gamma_1, \dots, \gamma_6, \tau_1, \tau_2, 0)$ ignoring $O(n^{-3/2})$ terms.

The proof for the three-step bootstrap goes similarly as that for the two-step bootstrap. First we note that $\tilde{z}_3(\eta(0, \lambda), \tau_1, \tau_2, \tau_3) \approx \Phi^{-1} \left\{ \int \Phi(\tilde{z}_2(\eta(0, v_\infty(0, z; \lambda, \tau_1)), \tau_2, \tau_3)) f(z) dz \right\}$, and that $\tilde{z}_2(\eta(0, v_\infty(0, z; \lambda, \tau_1)), \tau_2, \tau_3) = (\lambda + z\tau_1)(\tau_2^2 + \tau_3^2)^{-1/2} + O(n^{-1/2})$. Then $\tilde{z}_3(\eta(0, \lambda), \tau_1, \tau_2, \tau_3)$ is expressed in the same form as (A.9) but using $a = \tau_1(\tau_2^2 + \tau_3^2)^{-1/2}$, $b = \lambda(\tau_2^2 + \tau_3^2)^{-1/2}$, and different A_r 's. A straightforward calculation shows that this is equivalent to $\zeta_3(\gamma_1, \dots, \gamma_6, \tau_1, \tau_2, \tau_3)$ ignoring $O(n^{-3/2})$ terms.

B Mathematica session.

This section explains briefly Shimodaira (2003), which is a computer program in *Mathematica* notebook document referred to as *Program* here. This program is available in the *Mathematica* notebook format, PDF, and HTML from the author. *Program* proves the

third-order accuracy of the bias-corrected p -value calculated by the three-step multiscale bootstrap resampling. This newly devised bootstrap method is described in the paper Shimodaira (2004) referred to as *Paper* here.

The document starting below has the same section structure as *Program* with a brief explanation. This helps us to find the appropriate results in *Program*. The section numbers of *Program* are indicated with asterisk (*) to avoid confusion. Notational differences between *Paper* and *Program* are also explained.

Program consists of three parts, “Exponential Family of Distributions,” “Tube-Coordinates and z_c -formula,” and “Bootstrap Methods.” Each part is an independent *Mathematica* session, and should be run separately. In the first two parts, the tensor notation is heavily used. The add-on package *MathTensor* is required to run the session by yourself. I have first hand-calculated the results of the first two parts involving tensor notation, and later used *MathTensor* to verify the results. The last part has been calculated only by *Mathematica*.

***Part I**

Exponential Family of Distributions

***1 Startup**

This section initializes the *Mathematica* session.

***1.0.1 packages**

Statistics‘ContinuousDistributions‘ and MathTensor are loaded.

***1.0.2 error messages**

***1.0.3 distribution functions**

$f[x]$, $F[x]$, and $Q[p]$ are the density function, the distribution function, and the quantile function, respectively, for the standard normal random variable. $F[x]$ and $Q[p]$ are denoted $\Phi(x)$ and $\Phi^{-1}(p)$, respectively, in *Paper*. $f[x]$ is also denoted as $f(x) = (2\pi)^{-1/2} \exp(-x^2/2)$ here.

*2 Normal distribution

*2.1 The moments of the multivariate normal distribution

*2.1.1 the central moments of the standard normal variable in one dimension

$$\text{intx2f}[n] = \int_{-\infty}^{\infty} x^{2n} f(x) dx = \frac{(2n)!}{2^n n!}$$

This gives 1, 3, 15, 105, 945, ..., for $n = 1, 2, 3, 4, 5, \dots$

*2.1.2 define tensors

*2.1.3 the central moments for the multivariate case

Let $x = (x_a)$ denote a multivariate normal random vector with mean 0 and covariance identity. Then, the central moments, $\alpha_{ab} = E(x_a x_b)$, $\alpha_{abcd} = E(x_a x_b x_c x_d)$, and $\alpha_{abcdef} = E(x_a x_b x_c x_d x_e x_f)$ are given by `kd2[a,b]`, `kd4[a,b,c,d]`, and `kd6[a,b,c,d,e,f]`, respectively. They satisfy, for example, $\alpha_{112222} = E(x_1^2 x_2^4) = \text{intx2f}[1]\text{intx2f}[2] = 3$.

*2.2 The expectation of the exponential of polynomial functions

*2.2.1 central case

Let $\text{poly}(x)$ be a polynomial of x ,

$$\text{poly}(x) \approx a0 + a1^a x_a + a2^{ab} x_a x_b + a3^{abc} x_a x_b x_c + a4^{abcd} x_a x_b x_c x_d,$$

where $a0$ is $O(1)$, $a1, a2, a3$ are $O(n^{-1/2})$, and $a4$ is $O(n^{-1})$. We use ' \approx ' to indicate equivalence up to $O(n^{-1})$ terms ignoring the error of $O(n^{-3/2})$. The polynomial is expressed in *Program* as

$$\text{poly}(x) = a0 + o(a1^a x_a + a2^{ab} x_a x_b + a3^{abc} x_a x_b x_c) + o^2 a4^{abcd} x_a x_b x_c x_d,$$

where the o indicates a $O(n^{-1/2})$ term, and o^2 indicates a $O(n^{-1})$ term. Then,

$$\log E \{ \exp(\text{poly}(x)) \} \approx \text{logeexppolyb0}.$$

*2.2.2 noncentral case

When $E(x_a) = b_a$, we obtain

$$\log E \{ \exp(\text{poly}(x)) \} \approx \text{logeexppoly}.$$

*3 Exponential family

*3.1 The standard form

*3.1.1 simplification functions

*3.1.2 define tensors

*3.1.3 the log of the density function

Let $y = (y_a)$ be a multivariate random variable of dimension \mathbf{dim} , and the density function is specified by

$$f(y; \theta) = \exp(\theta^a y_a - h(y) - \psi(\theta)),$$

which corresponds to eq. (7.1) of *Paper* given below

$$\exp(\theta^i y_i - h(y) - \psi(\theta)).$$

The expression is given in $\log f(y; \theta) = \mathbf{logdensity}$ in *Program*. The dimension is denoted p in *Paper*, but it is denoted either \mathbf{dim} or $\mathbf{9}$ in *Program*; see Table 1. So $y = (y_1, \dots, y_9)$, $\theta = (\theta^1, \dots, \theta^9)$ here. We made $\mathbf{dim}=9$ only for a technical reason of *MathTensor*, and our calculation is independent of this choice. The indices to run $1, \dots, p$ in *Paper* are i, j, \dots , but those to run $1, \dots, 9$ in *Program* are $\mathbf{a}, \mathbf{b}, \dots$ for free indices, and $\mathbf{p}, \mathbf{q}, \dots$ for dummy indices. It should be noted that the indices to run $1, \dots, p-1$ in *Paper* are a, b, \dots , but those to run $1, \dots, 8$ in *Program* are $\mathbf{a}', \mathbf{b}', \dots$ or $\mathbf{p}', \mathbf{q}', \dots$. These differences are quite confusing, but a restriction using *MathTensor*.

In the tensor notation, covariant and contravariant indices are distinguished. In other words, a subscript and a superscript are summed over their range if they are a matched pair of indices. *MathTensor* and *Program* follow this rule. In *Paper*, however, the summation convention takes place for a pair of the same indices irrespective of subscripts and superscripts. This does not give any difference in the calculation, because we formally set the metric matrix to be identity, and specify the metric explicitly by the matrix multiplication when necessary.

Table 1: Notations of the indices

<i>Paper</i>	<i>Program</i>	description
p	\mathbf{dim} or $\mathbf{9}$	dimensions of the parameter vector
i, j, \dots	$\mathbf{a}, \mathbf{b}, \dots$ and $\mathbf{p}, \mathbf{q}, \dots$	indices run over $1, \dots, p$ (=9)
a, b, \dots	$\mathbf{a}', \mathbf{b}', \dots$ and $\mathbf{p}', \mathbf{q}', \dots$	indices run over $1, \dots, p-1$ (=8)

The natural parameter vector is $\theta = (\theta^a)$, and the expectation parameter vector $\eta = (\eta_a)$ is defined by $\eta_a = E(y_a; \theta)$. The potential function $\phi(\eta)$ is defined by $\phi(\eta) = \max_{\theta} \{\theta^a \eta_a - \psi(\theta)\}$, and the two parameterization are related to each other by $\eta_a = \partial\psi/\partial\theta^a$ and $\theta^a = \partial\phi/\partial\eta_a$. Without loss of generality, we assume

$$\left. \frac{\partial\phi}{\partial\eta_a} \right|_0 = 0, \quad \left. \frac{\partial^2\phi}{\partial\eta_a\partial\eta_b} \right|_0 = \delta^{ab} = \text{Kdelta}[a, b].$$

For higher order derivatives of ϕ at $\eta = 0$, we denote

$$\phi^{abc} = \left. \frac{\partial^3\phi}{\partial\eta_a\partial\eta_b\partial\eta_c} \right|_0 = o\phi\mathfrak{3}^{abc}, \quad \phi^{abcd} = \left. \frac{\partial^4\phi}{\partial\eta_a\partial\eta_b\partial\eta_c\partial\eta_d} \right|_0 = o^2\phi\mathfrak{4}^{abcd},$$

where the o indicates a $O(n^{-1/2})$ term, and o^2 indicates a $O(n^{-1})$ term.

*3.2 The expression of $\psi(\theta)$ in terms of η

*3.2.1 derivation

*3.2.2 result

$$\psi(\theta) \approx \psi(0) + \frac{1}{2}\eta_p\eta_p + \frac{1}{3}\eta_p\eta_q\eta_r\phi^{pqr} + \frac{1}{8}\eta_p\eta_q\eta_r\eta_s\phi^{pqrs} = \text{psieta},$$

which corresponds to eq. (A.1). The indices p, q, \dots are dummy indices to run $1, \dots, 9$ in *Program*.

*3.3 The expression of $h(y)$ in terms of ϕ derivatives

*3.3.1 derivation

*3.3.2 result

$$h(y) \approx \frac{1}{2}\text{dim}\log(2\pi) - \psi(0) + \frac{1}{2}y_p y_p - \frac{1}{2}y_p \phi^{pqq} + \frac{1}{6}y_p y_q y_r \phi^{pqr} - \frac{1}{6}(\phi^{pqr})^2 + \\ \frac{1}{4}y_p y_q \phi^{prs} \phi^{qrs} + \frac{1}{8}\phi^{ppqq} - \frac{1}{4}y_p y_q \phi^{pqrr} + \frac{1}{24}y_p y_q y_r y_s \phi^{pqrs} = \text{hinyphi},$$

which corresponds to eq. (A.2).

*3.4 The canonical form

*3.4.1 the summary of the previous sections

*3.4.2 result

Using the above expressions for $\psi(\theta)$ and $h(y)$, we obtain the expression for the density function using η -parameter.

$$\log f(y; \eta) = \text{logdensityy}.$$

The metric, i.e., the second derivative of ϕ , evaluated at a general point η is given by

$$\frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b} = \text{phi2eta}.$$

***Part II**

Tube-Coordinates and z_c -formula

***4 Startup**

This section initializes the *Mathematica* session.

***4.0.3 packages**

***4.0.4 error messages**

***4.0.5 distribution functions**

***5 Exponential family**

***5.1 The expectation of the exponential of a polynomial function of the normal vector**

***5.1.1 define tensors**

***5.1.2 logexpoly**

This is a result of Section *2.2.

***5.2 The canonical form of the density function**

***5.2.1 define tensors**

***5.2.2 logdensityy**

This is a result of Section *3.4.

***5.2.3 phi2eta**

This is a result of Section *3.4.

*6 Tube-coordinates

*6.1 Preliminary

*6.1.1 indices

*6.1.2 simplification functions

*6.1.3 define tensors

*6.2 The coordinates around the smooth surface

*6.2.1 smooth surface

Let $u = (u_{a'}) = (u_1, \dots, u_8)$ parameterize a surface in 9-dimensional space. The surface $\partial\mathcal{R} = \{\eta(u)\}$ is specified by

$$\eta_{a'}(u) = u_{a'}, \quad \eta_9(u) \approx -od^{a'b'} u_{a'} u_{b'} - o^2 e^{a'b'c'} u_{a'} u_{b'} u_{c'},$$

where the curvature matrix $od^{a'b'}$ is $O(n^{-1/2})$, and $o^2 e^{a'b'c'}$ is $O(n^{-1})$.

*6.2.2 tangent vectors

The b -th element of the a' -th tangent vector of $\partial\mathcal{R}$ at $\eta(u)$ is

$$B_b^{a'} = \frac{\partial \eta_b(u)}{\partial u_{a'}}$$

for $a' = 1, \dots, 8$, and $b = 1, \dots, 9$. The expressions are given in `foo3` and `foo4`, respectively, for $b = b'$ and $b = 9$. They are obtained by using the differential operator `difa` defined in Section *6.1.2. The metric for the tangent vectors is

$$\phi^{a'b'}(u) = \left. \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \right|_{\eta(u)} B_p^{a'}(u) B_q^{b'}(u) = \text{phi2bu}.$$

*6.2.3 the normal vector

The a -th element of the normal vector at $\eta(u)$ is B_a^9 for $a = 1, \dots, 9$. The expressions are given in `foo15` and `foo16`, respectively, for $a = a'$ and $a = 9$. B_a^9 is orthogonal to the tangent vectors with respect to the metric defined by the second derivative of $\phi(\eta)$, and it has the unit length directing away from the region \mathcal{R} .

*6.2.4 (u, v) -coordinate system

We define the reparameterization $\eta \leftrightarrow (u, v)$ by

$$\eta_a(u, v) = \eta_a(u) + B_a^9(u)v, \quad a = 1, \dots, 9,$$

where v is a scalar parameter. The expressions of $\eta_a(u, v)$ are given in `foo21` and `foo22`, respectively, for $a = a'$ and $a = 9$.

*6.3 Change of variables

*6.3.1 Jacobian

The Jacobian of the change of variables $\eta \leftrightarrow (u, v)$ is

$$J = \det \left(\frac{\partial \eta(u, v)}{\partial (u, v)} \right).$$

The asymptotic expression of $\log J$ in terms of (u, v) is given in `logdetJ`. This has been obtained in Lemma 8 of Section A.1 using a sophisticated argument, but here `logdetJ` is obtained more directly from the definition using *MathTensor*.

*6.3.2 density function $f(u, v|v0)$

The random vector y is also represented in (u, v) -coordinates. The density function $f(u, v|v0)$ is expressed by `logdensityuv` with the true parameter vector $\eta = (0, \dots, v0)$. This corresponds to eq. (7.4) of *Paper*. The scalar parameter $v0$ is denoted λ in Lemma 1 of *Paper*.

*7 z_c -formula

*7.1 Modified signed distance w

*7.1.1 define the modified signed distance as a series of v

Let us define a modified signed distance w by

$$w = v + \sum_{r=0}^{\infty} \text{cbr}[r]v^r + u_{a'} \sum_{r=0}^{\infty} \text{br}[a', r]v^r,$$

where the coefficients $\text{cbr}[r]$ and $\text{br}[a', r]$ are denoted by \bar{c}_r and \bar{b}_r^c , respectively, in eq. (7.8) of *Paper*. We assume that $\text{cbr}[0]$ and $\text{cbr}[2]$ are $O(n^{-1/2})$, and $\text{cbr}[1]$, $\text{cbr}[3]$, and all $\text{br}[a', r]$ are $O(n^{-1})$. The other $\text{cbr}[r]$ with $r \geq 4$ are all $O(n^{-3/2})$.

The inverse series specifies

$$v = w - \sum_{r=0}^{\infty} \text{cr}[r]w^r - u_{a'} \sum_{r=0}^{\infty} \text{br}[a', r]w^r = \mathbf{vinuw},$$

where $\text{cr}[r]$ has the same order as $\text{cbr}[r]$. Taking into account the magnitude of the coefficients, the expression is actually given in

$$\mathbf{vinuw} = w - o(\text{cr}[0] + w^2\text{cr}[2]) - o^2(\text{cr}[1] + w^3\text{cr}[3] + u_{a'}\text{br}^{a'})$$

in *Program*, where $\text{br}^{a'}$ indicates the $O(n^{-1})$ polynomial functions of w . The relation between these two sets of coefficients are given in **rule47**.

*7.1.2 density function of w

The joint density function of (u, w) is $f(u, w|v0)$. The asymptotic expression is given in $\log f(u, w|v0) = \mathbf{logdensityw}$. The marginal density $f(w|v0) = \int f(u, w|v0) du$ is obtained by using **logeexppoly**, and the expression is given in $\log f(w|v0) = \mathbf{logdensityw}$. These expressions are found in the proof of Lemma 4 of *Paper*.

*7.1.3 cumulants of w

By applying **logeexppoly** to $\mathbf{logdensityw}$, we calculate $\log \int e^{wt} f(w; \lambda) dw = t\kappa_1 + \frac{t^2}{2}\kappa_2 + \frac{t^3}{6}\kappa_3 + \frac{t^4}{24}\kappa_4 + \dots$ to obtain $\mathbf{cumulantw} = \{\kappa_1, \kappa_2, \kappa_3, \kappa_4\}$, the cumulants of w .

*7.2 Distribution function of w

*7.2.1 Cornish-Fisher expansion (p.66 of Johnson and Kotz 1994)

The Cornish-Fisher expansion for the standardized random variable is taken from Johnson and Kotz (1994) as shown in **cfexpw**, and the same expansion for nonstandardized variable is obtained as shown in **cfexpw**.

*7.2.2 Cornish-Fisher expansion of w

By applying **cfexpw** to $\mathbf{cumulantw}$, we obtain

$$\mathbf{zformula} = \Phi^{-1}(\Pr\{W \leq w; v0\}).$$

This corresponds to the z_c -formula $z_c(\hat{w}; \lambda, \tau)$ with $\hat{w} = w$, $\lambda = v0$, and $\tau = 1$ obtained in Lemma 4 of *Paper*.

*7.2.3 z_c -formula using a simplified notation

The same expression as `zformula`, but without *MathTensor* notation, is given in `zform`. The following table shows the notational differences.

Table 2: Notations of the geometric quantities

<i>Paper</i>	<code>zformula</code>	<code>zform</code>
d^{aa}	$d_{p'}^{p'}$	Daa
$(d^{ab})^2$	$(d_{p'}^{q'})(d_{q'}^{p'})$	Dab2
ϕ^{ppp}	$\phi 3^{999}$	P999
ϕ^{pppp}	$\phi 4^{9999}$	P9999
$(\phi^{app})^2$	$(\phi 3_{p'}^{99})(\phi 3^{99p'})$	P99a2
$d^{ab}\phi^{abp}$	$(d^{p'q'})(\phi 3_{p'q'}^9)$	DabP9ab
$(\phi^{abp})^2$	$(\phi 3_{p'}^9)(\phi 3_{q'}^9)^{p'}$	P9ab2
ϕ^{aapp}	$\phi 4_{p'}^{99p'}$	P99aa

*7.2.4 scaling by the factor τ

By applying the scaling rule described in Lemma 3 of *Paper*, we obtain the expression of $z_c(w; v0, \tau)$ in `zformulatau` or `zformtau`.

*7.3 Local coordinates at the projection

*7.3.1 the expression for the surface in the local coordinates

We consider a local coordinate $\Delta\eta = (\Delta\eta_a)$ around a point $\eta(u0, 0)$ on the surface, where $u0$ indicates any specified value of u . We will use a particular value of $u0$ specifying the projection of y onto the surface. This value is denoted \hat{u} in Lemma 5 of *Paper*. The change of variables $\eta \leftrightarrow \Delta\eta$ is specified by

$$\eta_a = \eta_a(u0, 0) + B_a^b(u0)\Delta\eta_b, \quad a = 1, \dots, 9.$$

The expression for $\eta_{a'}$ is given in `foo93` and that for η_9 is in `foo94`. The surface $\partial\mathcal{R}$ is now expressed as $\Delta\eta_9 = -\hat{d}^{a'b'}\Delta\eta_{a'}\Delta\eta_{b'} - \hat{e}^{a'b'c'}\Delta\eta_{a'}\Delta\eta_{b'}\Delta\eta_{c'}$, where the expression for $\hat{d}^{a'b'}$ is in `foo101` and that for $\hat{e}^{a'b'c'}$ is in `foo102`. These expressions are also found in the proof of Lemma 5.

*7.3.2 the expressions for the potential derivatives

The expression is given for

$$\left. \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \right|_{\eta = \eta(u_0) + B(u_0) \Delta \eta} B_p^a(u_0) B_q^b(u_0) = \text{foo114}[\mathbf{a}, \mathbf{b}].$$

*7.3.3 Geometric quantities at the projection

By comparing both sides of

$$\text{foo114}[\mathbf{a}, \mathbf{b}] = \hat{\phi}^{ab} + \hat{\phi}^{abc} \Delta \eta_c + \frac{1}{2} \hat{\phi}^{abcd} \Delta \eta_c \Delta \eta_d + \dots,$$

we obtain the expressions for $\hat{\phi}^{ab}$, $\hat{\phi}^{abc}$, and $\hat{\phi}^{abcd}$ as shown in `foo121`. The expression for the inverse matrix of the metric $\hat{\phi}_{a'b'} = (\hat{\phi}^{a'b'})^{-1}$ is shown in `foo131`, and it is used for $\hat{\phi}_{a'b'} \hat{a}^{a'b'} = \text{foo132}$.

*7.3.4 z_c -formula

The z_c -formula evaluated by taking $\eta(u_0, 0)$ as the origin of the local coordinates is shown in `zformulau0` or `zformulatauu0`. They correspond to $z_c(w; u_0, v_0, 1)$ and $z_c(w; u_0, v_0, \text{tau})$ in the notation of Lemma 5 of *Paper*. From the expressions, we observe that they depend on u_0 only linearly by ignoring $O(n^{-3/2})$ terms, and the magnitude is $O(n^{-1})$.

*Part III

Bootstrap Methods

*8 Startup

This section initializes the *Mathematica* session.

*8.0.5 packages

*8.0.6 error messages

*8.0.7 distribution functions

*9 Asymptotic Analysis of Bootstrap Methods

This section calculates the distribution functions of z -values appearing in several bootstrap methods for showing their asymptotic accuracies.

*9.1 Preliminary

*9.1.1 simplification functions

*9.1.2 zc-formula

$\text{zc}[\mathbf{w}, \{c_0, c_1, c_2, c_3\}, v_0, \text{tau}] = \text{zformtau}$ is $z_c(w; v_0, \text{tau}) = \Phi^{-1}(\Pr\{W \leq w; v_0, \text{tau}\})$, where u_0 is assumed zero. The coefficients $\{c_0, c_1, c_2, c_3\}$ specify the modified signed distance w , where $c_0 = \text{cr}[0], \dots, c_3 = \text{cr}[3]$ in the notation of zformtau . We do not need to use the more general zformtauu_0 in which $u_0 \neq 0$, because the u_0 terms contribute only $O(n^{-3/2})$ in the results of our calculation below.

*9.1.3 modified signed distance

Here we write $cb_0 = \text{cbr}[0], \dots, cb_3 = \text{cbr}[3]$. There are relations between $\{cb_0, \dots, cb_3\}$ and $\{c_0, \dots, c_3\}$, and cb2cc calculates the latter from the former.

*9.2 The pivot and some existing bootstrap methods

*9.2.1 pivot statistic

The pivot is defined as

$$\hat{z}_\infty(y) = -\Phi^{-1}(\Pr\{V \geq \hat{v}; u_0 = \hat{u}, v_0 = 0\})$$

in Section 7.5 of *Paper*, where (\hat{u}, \hat{v}) is the tube-coordinates of y . This is denoted as $\text{z8}[\mathbf{v}] = \text{zc}[\mathbf{v}, \{0, 0, 0, 0\}, 0, 1]$ in *Program* for $\hat{u} = u_0 = 0, \hat{v} = \mathbf{v}$. The $\hat{z}_q(y)$ in Lemma 6 of *Paper* is denoted $\text{zq}[v] = \text{z8}[v] + o(q_0 + q_2v^2) + o^2(q_1v + q_3v^3)$. zq2qq calculates $\text{qq} = \{q_0, q_1, q_2, q_3\}$ from any z -value. cb_r 's and c_r 's for z8 are in cbzq and czqq , respectively. The distribution function of $\text{zq}[V]$ is obtained as $\Pr\{\text{zq}[V] \leq w; v_0, \text{tau}\} = \Phi\{\text{zfqzq}[\mathbf{w}, \{q_0, q_1, q_2, q_3\}, v_0, \text{tau}]\}$. We observe that $\text{zfqzq}[\mathbf{w}, \{0, 0, 0, 0\}, 0, 1] = w$, and thus the distribution function of z8 under $v_0 = 0$ is $\Pr\{\text{Z8} \leq w; 0, 1\} \approx \Phi(w)$.

*9.2.2 bootstrap probability

The multiscale bootstrap probability for the scale τ is

$$\tilde{\alpha}_1(y, \tau) = \Pr\{V \leq 0; u_0 = \hat{u}, v_0 = \hat{v}, \tau\}$$

The corresponding z -value is denoted $\tilde{z}_1(y, \tau) = -\Phi^{-1}(\tilde{\alpha}_1(y, \tau)) = -z_c(0; \hat{u}, \hat{v}, \tau)$ in the notation of Section 7.6 of *Paper*. For $y = \eta(\hat{u}, \hat{v})$ with $\hat{u} = u_0 = 0$ and $\hat{v} = \mathbf{v}$, and $\tau = \text{tau1}$, the z -value is expressed as

$$\text{z1}[\mathbf{v}, \text{tau1}] = \text{zc}[0, \{0, 0, 0, 0\}, \mathbf{v}, \text{tau1}]$$

in *Program*. For $\text{tau1} = 1$, we define $\mathbf{z0}[\mathbf{v}] = \mathbf{z1}[\mathbf{v}, 1]$, corresponding to $\hat{z}_0(y)$ in *Paper*. For general value of tau1 , $\mathbf{w1} = \text{tau1} \mathbf{z1}[\mathbf{v}, \text{tau1}]$ is regarded as another w with \mathbf{cb}_r 's being $\mathbf{cbw1}$ and \mathbf{c}_r 's being $\mathbf{ccw1}$, and the distribution function is expressed as $\Pr\{W1 \leq w; v0, \text{tau}\} = \Phi(\mathbf{zfw1})$ under the scale tau . For $\text{tau} = 1$ and $\text{tau1} = 1$, we have $\Pr\{\hat{Z}_0 \leq w; v0, \text{tau} = 1\} = \Phi(\mathbf{zfvz0}[w, v0])$, which becomes $\mathbf{zfvz0}[w, 0] = w + O(n^{-1/2})$ under $v0 = 0$, showing the first-order accuracy of $\mathbf{z0}[\mathbf{v}]$.

*9.2.3 double bootstrap

The z -value of the double bootstrap probability is

$$\mathbf{zd}[v] = -\Phi^{-1}(\Pr\{\hat{Z}_0 \leq \hat{z}_0(v); v0 = 0\}),$$

corresponding to $\hat{z}_{\text{double}}(y)$ in Section 7.6 of *Paper*. We observe that $\mathbf{zd}[\mathbf{v}] = \mathbf{z8}[\mathbf{v}]$, showing the third-order accuracy of the double bootstrap probability.

*9.2.4 two-level bootstrap

The ABC formula is given in `abcformula[v, ac]`. The z -value corresponding to the two-level bootstrap corrected p -value is calculated in `za[v]`. Its q_i 's are in `qqza`. The distribution function of `za[v]` under $\text{tau} = 1$ is

$$\Pr\{\mathbf{za}[V] \leq w; v0, 1\} = \Phi(\mathbf{zfvzq}[w, \text{qqza}, v0, 1]),$$

which becomes $\Phi(w) + O(n^{-1})$ for $v0 = 0$, showing the second-order accuracy of the two-level bootstrap.

*9.3 Multistep-multiscale bootstrap method

*9.3.1 a generalization of the pivot

The pivot `z8[v]` is generalized to define

$$\mathbf{z8}[\mathbf{v}, v0, \text{tau}] = \mathbf{zc}[\mathbf{v}, \{0, 0, 0, 0\}, v0, \text{tau}],$$

which is denoted $\hat{z}_\infty(0, v; v0, \text{tau})$ in the proof of Lemma 7 of *Paper*. `z8[v, v0, tau]` reduces to `z8[v]` when $v0 = 0$ and $\text{tau} = 1$. We show that

$$\Pr\{\mathbf{z8}[V, v0, \text{tau}] \leq w; v0, \text{tau}\} \approx \Phi(w).$$

The inverse function of `z8[v, v0, tau] = z` in terms of `v` is also defined here so that `v8[z, v0, tau] = v`.

*9.3.2 some useful formula for normal integration

Let $\text{func}[z] = (az + b) + \text{rem}[z]$, where $\text{rem}[z]$ is a polynomial function of z with magnitude $O(n^{-1/2})$. Then

$$\Phi^{-1} \left\{ \int_{-\infty}^{\infty} \Phi(\text{func}[z]) f[z] dz \right\} \approx \text{ddint}[a, b, \text{func2dd}[a, b, \text{rem}, z], z].$$

*9.3.3 two-step multiscale bootstrap

Using ddint function defined above, we calculate

$$\begin{aligned} \mathbf{z2}[\mathbf{v0}, \mathbf{tau1}, \mathbf{tau2}] &\approx \Phi^{-1} \left\{ \int_{-\infty}^{\infty} \Phi(\mathbf{z1}[v, \mathbf{tau2}]) f[v, v0, \mathbf{tau1}] dv \right\} \\ &\approx \Phi^{-1} \left\{ \int_{-\infty}^{\infty} \Phi(\mathbf{z1}[\mathbf{v8}[z, v0, \mathbf{tau1}], \mathbf{tau2}]) f[z] dz \right\}, \end{aligned}$$

where $\mathbf{z2}[\mathbf{v0}, \mathbf{tau1}, \mathbf{tau2}]$ corresponds to $\tilde{z}_2(y, \tau_1, \tau_2)$ in eq. (7.18) of *Paper* for $y = \eta(\hat{u}, \hat{v})$ with $\hat{u} = u0 = 0$ and $\hat{v} = v0$. This is the z -value of the twostep-multiscale bootstrap probability.

*9.3.4 three-step multiscale bootstrap

Similarly, we calculate the z -value of the threestep-multiscale bootstrap probability defined by

$$\begin{aligned} \mathbf{z3}[\mathbf{v0}, \mathbf{tau1}, \mathbf{tau2}, \mathbf{tau3}] &\approx \Phi^{-1} \left\{ \int_{-\infty}^{\infty} \Phi(\mathbf{z2}[v, \mathbf{tau2}, \mathbf{tau3}]) f[v, v0, \mathbf{tau1}] dv \right\} \\ &\approx \Phi^{-1} \left\{ \int_{-\infty}^{\infty} \Phi(\mathbf{z2}[\mathbf{v8}[z, v0, \mathbf{tau1}], \mathbf{tau2}, \mathbf{tau3}]) f[z] dz \right\}. \end{aligned}$$

This gives the expression of $\tilde{z}_3(y, \tau_1, \tau_2, \tau_3)$ with $\hat{u} = 0$ and $\hat{v} = v0$.

*9.3.5 simplifying $\mathbf{z3}$ and $\mathbf{z8}$

The six geometric quantities $\gamma_1, \dots, \gamma_6$ defined in Lemma 7 of *Paper* are denoted by $\mathbf{G1}, \dots, \mathbf{G6}$ here. The scaling parameters s_1, \dots, s_4 in eq. (5.5) of *Paper* are now denoted $\mathbf{S1}, \dots, \mathbf{S4}$. We define $\mathbf{Z3G}$ and $\mathbf{Z8G}$ in terms of $\mathbf{G1}, \dots, \mathbf{G6}, \mathbf{S1}, \dots, \mathbf{S4}$, and show that $\mathbf{Z3G} \approx \mathbf{z3}[\mathbf{v}, \mathbf{tau1}, \mathbf{tau2}, \mathbf{tau3}]$ and $\mathbf{Z8G} \approx \mathbf{z8}[\mathbf{v}]$. In fact, $\mathbf{Z3G}$ and $\mathbf{Z8G}$, respectively, are $\zeta_3(\gamma_1, \dots, \gamma_6, \tau_1, \tau_2, \tau_3)$ of eq. (5.5) and $\hat{z}_3(y)$ of eq. (5.6) defined in Section 5 of *Paper*.

We have shown earlier that $\tilde{z}_3 = \mathbf{z3}$ is the z -value of the threestep-multiscale bootstrap probability, and that $\hat{z}_\infty = \mathbf{z8}$ is the third-order accurate pivot statistic. Therefore, the equivalence $\zeta_3 = \mathbf{Z3G} \approx \mathbf{z3} = \tilde{z}_3$ and $\hat{z}_3 = \mathbf{Z8G} \approx \mathbf{z8} = \hat{z}_\infty$ proves the third-order accuracy

of the threestep-multiscale bootstrap corrected p -value, in which G_1, \dots, G_6 are estimated from $Z3G$ and used to calculate $Z8G$. Should we note the notational difference between \tilde{z}_3 and \hat{z}_3 ; namely, the z -value of the threestep-multiscale bootstrap probability and the z -value of the threestep-multiscale bootstrap corrected p -value, respectively.

References

- JOHNSON, N. L., KOTZ, S. AND BALAKRISHNAN, N. (1994). *Continuous univariate distributions. Vol. 1.* John Wiley & Sons Inc., New York, second edition. A Wiley-Interscience Publication.
- KURIKI, S. AND TAKEMURA, A. (2000). Shrinkage estimation towards a closed convex set with a smooth boundary. *J. Multivar. Anal.* **75**, 79–111.
- SHIMODAIRA, H. (2003). Asymptotic analysis of the bootstrap methods. *Mathematica notebook document* (<http://www.is.titech.ac.jp/~shimo>), Department of Mathematical and Computing Sciences, Tokyo Institute of Technology, Tokyo, Japan.
- SHIMODAIRA, H. (2004). Approximately unbiased tests of regions using multistep-multiscale bootstrap resampling. Research Reports B-402, Department of Mathematical and Computing Sciences, Tokyo Institute of Technology, Tokyo, Japan.
- WEYL, H. (1939). On the volume of tubes. *American Journal of Mathematics* **61**, 461–472.