Higher-order accuracy of multiscale-double bootstrap for testing regions

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Abstract: We consider hypothesis testing for the null hypothesis being represented
as an arbitrary-shaped region in the parameter space. We compute an approximate
p-value by counting how many times the null hypothesis holds in bootstrap replicates.
This frequency, known as bootstrap probability, is widely used in evolutionary biology,
but often reported as biased in the literature. Based on the asymptotic theory of
bootstrap confidence intervals, there have been some new attempts for adjusting the
bias via bootstrap probability without direct access to the parameter value. One such an
test is the double bootstrap which adjusts the bias by bootstrapping the bootstrap
probability. Another new attempt is the multiscale bootstrap which is similar to the
m-out-of-n bootstrap but very unusually extrapolating the bootstrap probability to
m = −n. In this paper, we employ these two attempts at the same time, and call the
new procedure as multiscale-double bootstrap. By focusing on the multivariate normal
model, we investigate higher-order asymptotics up to fourth-order accuracy. Geometry
of the region plays important roles in the asymptotic theory. It was known in the
literature that the curvature of the boundary surface of the region determines the bias
of bootstrap probability. We found out that the “curvature of curvature” determines the
remaining bias of double bootstrap. The multiscale bootstrap removes these biases. The
multiscale-double bootstrap is fourth order accurate with coverage probability erring
only \( O(n^{-2}) \), and it is robust against computational error of parameter estimation
used for generating bootstrap replicates from the null distribution.

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unbiased tests, fourth-order accuracy, scaling-law, mean curvature, bias correction.

1. Introduction

We would like to compute approximate p-values by bootstrap methods for testing null hy-
pothesis \( H_0 : \mu \in H \) against alternative \( H_1 : \mu \notin H \) for a \( q + 1 \) (\( \geq 2 \))
dimensional unknown parameter vector \( \mu \in \mathbb{R}^{q+1} \) and an arbitrary-shaped region \( H \subset \mathbb{R}^{q+1} \). This is the prob-
lem of regions discussed in Efron, Halloran and Holmes (1996) and Efron and Tibshirani
(1998), where the geometry of the shape of \( H \) plays important roles. Their geometric argu-
mint is based on the bias-corrected (BC) bootstrap confidence interval of Efron (1985) for
the multivariate normal model

\[ Y \sim N_{q+1}(\mu, I_{q+1}) \]

with mean \( \mu \) and covariance identity matrix \( I_{q+1} \). Similar geometric argument is found in
Efron (1987), DiCiccio and Efron (1992), and Shimodaira (2004) for exponential family of
distributions up to terms of \( O(n^{-1}) \). We focus on the multivariate normal model (1) in this

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A simple example is the case of spherical region in Efron and Tibshirani (1998). Consider $n$ independent random variables $X_1, \ldots, X_n \sim N_q(\eta, I_p)$, and the null hypothesis $|\eta| \leq 1$, where $|\eta|^2 = \eta_1^2 + \cdots + \eta_p^2$. The problem is also described in a transformed variable $Y = \sqrt{n}X$ with mean $\mu = \sqrt{n}\eta$ so that the region is $H = \{\mu : |\mu| \leq \sqrt{n}\}$. The dependency on $n$ is implicit in our notation. This example is simple enough to compute the exact p-value as $P(|Y|^2 \geq |y|^2)$ by knowing that $|Y|^2$ follows $\chi^2_{p+1}$, the chi-square distribution with degrees of freedom $p + 1$, of non-centrality $|\mu|^2$. However, it is not so easy to compute the exact p-value for an arbitrary-shaped region $H$.

Having an observation $y \in \mathbb{R}^{p+1}$ of $Y$, we may generate many replicates of $Y$ by the parametric bootstrap

$$Y^* \sim N_{q+1}(y, \sigma^2 I_{q+1})$$

for some $\sigma^2 > 0$. This corresponds to the non-parametric “m-out-of-n” bootstrap of Bickel, Götze and van Zwet (1997) and Politis and Romano (1994) with $\sigma^2 = n/m$. For the spherical example, we may compute $Y^* = \sqrt{n}(X_1^* + \cdots + X_n^*)/m$ by resampling $\{X_1^*, \ldots, X_n^*\}$ with replacement from $\{x_1, \ldots, x_n\}$. In this paper, we do not pursue the non-parametric bootstrap, but focus on (2) for extending the asymptotic theory of Efron (1985).

Generating many $Y^*$’s, we count how many times they fall in $H$. This frequency is called as bootstrap probability (BP) and it has been used extensively since Felsenstein (1985) for approximating the p-value of testing phylogenetic trees in evolutionary biology. It is also named “empirical strength probability” in Liu and Singh (1997). Although the BP works as an approximate p-value in the frequentist sense, it is often reported as biased and there have been some attempts for improving the accuracy: Hillis and Bull (1993), Felsenstein and Kishino (1993), Newton (1996), Efron, Halloran and Holmes (1996), Efron and Tibshirani (1998), Shimodaira (2002, 2004, 2008).

Assuming sufficiently large number of replicates, we define the BP as

$$BP_{\sigma^2}(H|y) = P_{\sigma^2}(Y^* \in H|y),$$

where $P_{\sigma^2}(\cdot|y)$ indicates the probability with respect to (2). The variance is usually $\sigma^2 = 1$ and we simply denote BP or $BP(H|y)$ for $BP_1(H|y)$. BP is interpreted as the Bayesian posterior probability of $H$ under (1), because the posterior distribution is $\mu|y \sim N_{p+1}(y, I_{p+1})$ for the improper uniform prior distribution.

For a specified significance level $0 < \alpha < 1$, we will reject $H_0$ if $BP < \alpha$. It follows from eq. (2.22) of Efron and Tibshirani (1998) that the rejection probability is expressed as

$$P\left(BP(H|Y) < \alpha\right) = \Phi(z_\alpha + 2\gamma_1) + O(n^{-1})$$

for $\mu \in \partial H$, where $\gamma_1 = O(n^{-1/2})$ is the mean curvature of $\partial H$ at $\mu$ in terms of differential geometry. Here $\partial H$ denotes the boundary surface of the region $H$, $\Phi(\cdot)$ is the cumulative distribution function of $N(0, 1)$, and $z_\alpha = \Phi^{-1}(\alpha)$. A generalization of (3) will be proved later in Theorem 5. The rejection probability of unbiased tests should be equal to $\alpha$ for $\mu \in \partial H$, and the bias is defined as the deviation of rejection probability from $\alpha$. According to (3), the bias of BP is determined mostly by the mean curvature, which is zero, say, if $\partial H$ is flat. More generally, the mean curvature is zero everywhere on a “minimal surface” that locally minimizes its area like soap membranes. We may reject $H_0$ too much (large type-I error and many false positives) if the curvature is positive, and reject $H_0$ too little.
The bootstrap iteration is a general idea applicable to a wide range of problems for improving accuracy, and it has been applied to bootstrap confidence intervals of a real parameter; Hall (1986), Beran (1987), Loh (1987), Hinkley and Shi (1989), Martin (1990), Hall (1992), Efron and Tibshirani (1993), Newton and Geyer (1994), Lee and Young (1995), DiCiccio and Efron (1996), Hall and Maesono (2000). From the duality of confidence intervals and hypothesis testing, we may compute a $p$-value from the iterated bootstrap confidence intervals of a real parameter, say, $\|\mu\|$ for the spherical example. However, additional consideration is needed for computing the $p$-value only from the frequency of $\{\|y^*\| \leq \sqrt{n}\}$ without access to the bootstrap distribution of $\|y^*\|$. Efron and Tibshirani (1998) applied the bootstrap iteration to BP for adjusting the bias, and called the bias-corrected BP as a calibrated confidence level. In this paper, we call it as double bootstrap probability (DBP).

Similar to the bias of BP, the remaining bias of DBP is again interpreted as a geometric quantity of $\partial H$. Let $\beta_3 = O(n^{-3/2})$ be the “mean curvature of the mean curvature” of $\partial H$. We found that $\beta_3$ determines the bias of DBP. In fact, the rejection probability is

$$P\left(DBP(H|Y) < \alpha\right) = \Phi(z_\alpha - 2\beta_3) + O(n^{-2})$$

as shown in Theorem 6. Related results are given in Hall (1992) and Lee and Young (1995) for the coverage probability of the iterated bootstrap confidence intervals under the smooth function model. We can tell from (4) that DBP is very accurate for the spherical example, because $\beta_3 = 0$ for spheres. For constant-mean-curvature surfaces, such as plane, cylinder, sphere, or intuitively soap bubbles, we have always $\beta_3 = 0$, and DBP is very accurate. For other surfaces, however, the magnitude of $\beta_3$ can be large.

In this paper, we discuss several bootstrap methods for improving the accuracy of BP. An approximately unbiased $p$-value is said to be $k$-th order accurate if the bias is $O(n^{-k/2})$ asymptotically. BP is only first order accurate, and DBP is third order accurate. We attempt improving BP and DBP via the multiscale bootstrap of Shimodaira (2002, 2004, 2008). A key idea is to change $\sigma^2$ in (2). We derive the scaling-law of BP and DBP with respect to $\sigma^2$, and extrapolate these values formally to $\sigma^2 = -1$, or $m = -n$ in the non-parametric bootstrap. The idea is analogous to the SIMEX, simulation-extrapolation, method for measurement error models of Cook and Stefanski (1994). It turns out that $\gamma_1$ in (3) and $\beta_3$ in (4) disappear as $\sigma^2$ approaching $-1$. Thus the multiscale bootstrap improves both BP and DBP; the bias-corrected BP is third-order accurate, and the bias-corrected DBP is fourth-order accurate. This is the main thrust of the paper. We will prove the main results in Section 5 after preparing geometric tools in Section 4.

The bias-corrected BP via multiscale bootstrap has been already used for testing phylogenetic trees in Shimodaira and Hasegawa (2001) and hierarchical clustering in Suzuki and Shimodaira (2006), and the hypothesis test is referred to as “approximately unbiased” (AU) test in the literature. For the newly proposed bias-corrected DBP, we call the procedure as multiscale-double bootstrap, and the hypothesis test as “double approximately unbiased” (DAU) test. This procedure is new and different from the two-step multiscale bootstrap of Shimodaira (2004) which adjusts AU without double-bootstrapping for exponential family of distributions.
2. Conventional testing procedures

For representing $H$, we use $(u, v)$ coordinates with $u = (u_1, \ldots, u_q) \in \mathbb{R}^q$ and $v \in \mathbb{R}$. Given a smooth function $h(u)$ of $u \in \mathbb{R}^q$, we specify a region as $\mathcal{R}(h) = \{(u, v) | v \leq -h(u), u \in \mathbb{R}^q\}$, and assume that $H = \mathcal{R}(h)$. The boundary surface $\partial H$ is denoted as $B(h) = \{(u, v) | v = -h(u), u \in \mathbb{R}^q\}$. For example, $h(u) = (h_0^2 + u^2/3)^{1/2}$ (5) with $q = 1$, $h_0 = 0.1$ is shown in Fig 1. The region with $h_0 > 0$ is related to the confidence limit of the product $\mu_1\mu_2$ discussed in Efron (1985), and the region with $h_0 \rightarrow 0$ is related to the multiple comparisons problem as mentioned later. Observing $y = (1/\sqrt{2}, \sqrt{8}/3) = (0.71, 1.63)$, say, we would like to evaluate the chance of $H_0$ being true. We will compute $p$-values by several methods as shown in Table 1. Results are also shown for $y = (3.18, 0.20)$. We occasionally come back to this example throughout the paper.

Let us look at likelihood ratio (LR) tests first. We consider null hypothesis $H'_0 : \mu \in \partial H$ against alternative $H'_1 : \mu \notin \partial H$. Since the log-likelihood function is simply $\ell(\mu; y) = -\frac{1}{2}\|y - \mu\|^2$, the maximum likelihood estimate for $\mu \in \mathbb{R}^{q+1}$ is $y$, and the restricted maximum likelihood estimate for $\mu \in \partial H$ is given by

$$\hat{\mu}(H|y) = \arg \min_{\mu \in \partial H} \|y - \mu\|.$$

By numerical optimization, we get $\hat{\mu}(H|y) = (0.12, -0.12)$ for $y = (0.71, 1.63)$, and the LR statistic is then $2\ell(y; y) - 2\ell(\hat{\mu}(H|y); y) = \|y - \hat{\mu}(H|y)\|^2 = 1.85^2 = 3.42$. The $p$-value is computed as $P(\chi^2_1 \geq 3.42) = 0.064$. 

![Fig 1. The two cases of observation y and restricted MLE $\hat{\mu}(H|y)$. Signed distances are indicated by dotted lines. The boundary surface $\partial H$ for (5) with $h_0 = 0.1$ is drawn by solid curve. The null hypothesis is represented as the region below the curve.](image-url)
However, the following two issues of LR tests are pointed out in Efron (1985) and Efron and Tibshirani (1998). (i) The LR test ignores the side of $\partial H$ in which $y$ lies. We can improve the LR test by replacing the alternative $H'_1$ by $H_1$. McCullagh (1984) introduced the signed LR statistic $\hat{\lambda} = \pm \sqrt{2} f(y; y) - 2\ell(\mu(H; y); y)$ with positive sign for $y \notin H$ and negative sign for $y \in H$. Efron (1985) called $\hat{\lambda} = \pm ||y - \mu(H)||$ as signed distance for the multivariate normal model. Since $\hat{\lambda} \sim N(0,1)$ under $H_0'$ asymptotically, the $p$-value for testing $H'_0$ against $H_1$ is computed as $1 - \Phi(1.85) = 0.032$, which is half of the $p$-value of the LR test. This one-sided test of $\hat{\lambda}$ has twice the power of the (two-sided) LR test. (ii) The LR test and the signed LR test are biased by $O(n^{-1/2})$. This bias is corrected by the Bartlett adjustment, which works in a way very similar to eliminating $\gamma_1$ from (3). Our bootstrap methods will compute $p$-values similar to the bias-corrected signed LR test.

For testing $H_0$ against $H_1$, we could construct a confidence set of $\mu$ as

$$S(y) = \{\mu \mid ||\mu - y||^2 \leq \chi^2_{2,1-\alpha}\},$$

where $\chi^2_{2,1-\alpha}$ is the upper $\alpha$ point of $\chi^2_2$. We will reject $H_0$ if the intersection of $S(y)$ and $H$ is empty. The $p$-value is computed as $P(\chi^2_2 \geq 3.42) = 0.181$. This method controls the type-I error for any $H$. However, it is very conservative and $p$-value is unnecessarily large, because $S(y)$ does not take account of the shape of $H$.

In the case of $h_0 = 0$, the multiple comparisons with the best (MCB) procedure of Hsu (1981) can be used for testing $H_0$ against $H_1$. Observing $\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3)$ from $\bar{X} \sim N_3(\eta, \Sigma/n)$ with $\eta = (\eta_1, \eta_2, \eta_3)$, we would like to know if $\eta_1$ is the largest among the three population means. MCB assumes the least favorable configuration $\eta_1 = \eta_2 = \eta_3$ for computing the null distribution of the test statistic $t = \sqrt{n} \max(\bar{x}_2 - \bar{x}_1, \bar{x}_3 - \bar{x}_1)$. The null hypothesis $\eta_1 \geq \max(\eta_2, \eta_3)$ is represented as the cone-shaped region $v \leq -|u|/\sqrt{3}$ by transformation $u = \sqrt{n/2}(\eta_3 - \eta_2)$ and $v = \sqrt{n/6}(\eta_2 + \eta_3 - 2\eta_1)$. For the two cases of $y$ in Table 1, the test statistic is actually the same value $t = 2.5$ and $p$-value is $P(T \geq t) = 0.069$. Since MCB is unbiased at $\mu = (0,0)$, i.e., the vertex of the cone, the $p$-value will be a reasonable value for $y = (0.71, 1.63)$. However, MCB becomes conservative as $\mu$ moves away from the vertex, and the $p$-value may be unnecessarily large for $y = (3.18, 0.20)$. MCB will be compared with bootstrap methods in the simulation study of Section 3.5.

| observation $y$ | (0.71, 1.63) | (3.18, 0.20) |
|-----------------|--------------|--------------|
| hypothesis $h_0$ | 0.1 | 0.0 | 0.1 | 0.0 |
| conventional testing procedures | | | |
| LR | 6.4 | 7.5 | 7.7 | 7.9 |
| signed LR | 3.2 | 3.8 | 3.8 | 3.9 |
| $S(y)$ | 18.1 | 20.5 | 20.8 | 21.0 |
| MCB | - | 6.9 | - | 6.9 |
| bootstrap methods | | | |
| BP | 1.8 | 2.0 | 3.8 | 3.8 |
| AU2 | 4.2 | 4.6 | 3.9 | 3.9 |
| AU3 | 5.5 | 6.2 | 3.7 | 3.7 |
| DBP | 4.8 | 6.1 | 3.9 | 4.0 |
| DAU | 5.4 | 6.9 | 3.7 | 3.7 |
3. Bootstrap Methods

3.1. Asymptotic theory of surfaces

We assume that all the axes in \((u, v)\) coordinates are scaled by \(\sqrt{n}\) asymptotically as \(n \to \infty\). This is easily verified for the spherical example of Section 1. We only have to assume that \(H\) is represented as \(R(h)\) in a neighborhood of a point of interest.

We consider the Taylor series of \(h(u)\) at \(u = 0\) as

\[
h(u) \simeq h_0 + h_1 u_i + h_{ij} u_i u_j + h_{ijk} u_i u_j u_k + h_{ijkl} u_i u_j u_k u_l,
\]

where \(\simeq\) denotes the equality correct up to \(O(n^{-3/2})\) erring \(O(n^{-2})\), and the summation convention such as \(h_{ij} u_i u_j = \sum_{i=1}^{q} \sum_{j=1}^{q} h_{ij} u_i u_j\) is used. Then, the second derivative

\[
h_{ij} = \frac{1}{2} \frac{\partial^2 h(u)}{\partial u_i \partial u_j}
\]

is \(O(n^{-1/2})\), because the numerator is \(O(\sqrt{n})\) and the denominator is \(O(n)\). Similarly, the \(k\)-th order derivatives are \(O(n^{-(k-1)/2})\), \(k \geq 2\). As \(n \to \infty\), all these derivatives approaches zero, and \(\partial H\) becomes a flat surface.

We can always assume that \(h_0 = 0\), \(h_i = 0\) by taking the origin \((0, 0)\) at a point on \(\partial H\) and the \(u_1, \ldots, u_q\) axes in directions tangent to \(\partial H\). These \((u, v)\) coordinates are used in eq. (2.10) of Efron and Tibshirani (1998) for representing \(H\). The mean curvature of \(\partial H\) at \((0, 0)\) is defined as

\[
\gamma_1 = \frac{1}{2} \frac{\partial^2 h(u)}{\partial u_i \partial u_i}
\]

The mean curvature of \(\partial H\) at \((u, \lambda h(u))\), denoted as \(\gamma_1(h, u),\) is defined similarly by taking the origin there. The asymptotic expression of \(\gamma_1(h, u)\) will be given later in Section 4.2.

The mean curvature of the mean curvature of \(\partial H\) at \(0, 0\) is then expressed as

\[
\beta_3 = \frac{1}{2} \frac{\partial^2 \gamma_1(h, u)}{\partial u_i \partial u_i}
\]

In the next sections, we will show asymptotic expansions of bootstrap methods. It is convenient for the argument there to assume \(h_0 = O(1)\) and \(h_i = O(n^{-1})\) by relaxing the assumptions of \(h_0 = 0\) and \(h_i = 0\). For \(\lambda_0 \in \mathbb{R}\), we assume that the observation is

\[
y = (0, \lambda_0 - h_0)
\]

in the \((u, v)\) coordinates. We assume \(\lambda_0 = O(1)\) for the local alternatives; in the spherical example, say, \(\eta\) approaches the boundary surface \(\|\eta\| = 1\) with distance \(O(n^{-1/2})\). Although \(u_i\) axes are slightly tilted from the tangent space, the signed distance is \(\lambda = \lambda_0(1 + O(h_i^2)) \simeq \lambda_0\), meaning that we can ignore the influence of \(h_i\).

We say that a smooth function \(h\) belongs to class \(S\) if it is expressed asymptotically as \((7)\) with coefficients

\[
h_0 = O(1), h_i = O(n^{-1}), h_{ij} = O(n^{-1/2}), h_{ijk} = O(n^{-1}), h_{ijkl} = O(n^{-3/2}).
\]

For \(h \in S\), we define the following quantities representing geometric properties of \(\partial H\) at \((0, -h(0))\),

\[
\gamma_1 = h_{ii} = O(n^{-1/2}), \quad \gamma_2 = h_{ij} h_{ij} = O(n^{-1}), \quad \gamma_3 = h_{ij} h_{jk} h_{ki} = O(n^{-3/2}), \quad \gamma_4 = h_{ijij} = O(n^{-3/2}).
\]
The first three quantities are also written as \(\gamma_1 = \text{tr}(D), \gamma_2 = \text{tr}(D^2), \gamma_3 = \text{tr}(D^3)\) using \(q \times q\) matrix \(D\) with elements \((D)_{ij} = h_{ij}\). Asymptotic expansions of bootstrap methods will be expressed up to \(O(n^{-3/2})\) terms by using only

\[
\begin{align*}
\beta_0 &= \lambda_0 = O(1), \quad \beta_1 = \gamma_1 - \lambda_0 \gamma_2 + \frac{1}{2} \lambda_0^2 \gamma_3 = O(n^{-1/2}), \\
\beta_2 &= 3\gamma_4 - \gamma_1 \gamma_2 - \frac{4}{3} \lambda_0^3 = O(n^{-3/2}), \quad \beta_3 = 6\gamma_4 - 2\gamma_1 \gamma_2 - 4\lambda_0^3 = O(n^{-3/2}).
\end{align*}
\]  

(11)

We will verify in Section 4.2 that the above definition of \(\beta_3\) in (11) is consistent with (8).

3.2. Asymptotic expansion of the bootstrap probability

Efron and Tibshirani (1998) showed the asymptotic expansion of \(\text{BP}(H|y)\) up to \(O(n^{-1})\) terms. We generalize their eq. (2.19) to include \(O(n^{-3/2})\) terms. For convenience, we use

\[\Phi(x) = 1 - \Phi(x) = \Phi(-x).\]

All the proofs of theorems are found in Appendix.

**Theorem 1** (Bootstrap probability). Consider \(y = (0, \lambda_0 - h_0)\) and the region \(H = R(h)\) for \(h \in S\). The bootstrap probability for \(\sigma^2 = 1\) is then expressed asymptotically as

\[\text{BP}(H|y) \simeq \Phi(\lambda_0 + \gamma_1 - \lambda_0 \gamma_2 + 3\gamma_4 - \gamma_1 \gamma_2 - \frac{4}{3}(1 - \lambda_0^3)\gamma_3).\]

(12)

Using the coefficients defined in (11), it becomes

\[\text{BP}(H|y) \simeq \Phi(\beta_0 + \beta_1 + \beta_2).\]

(13)

Efron and Tibshirani (1998) also showed a third-order accurate \(p\)-value. We generalize their eq. (2.17) to include \(O(n^{-3/2})\) terms. We will show later in Section 5.2 that the \(p\)-value defined below is fourth-order accurate.

\[\text{PV}(H|y) \simeq \Phi(\beta_0 - \beta_1 - \beta_2 + \beta_3).\]

(14)

Comparing (13) with (14), we find that \(\text{BP}\) differs from \(\text{PV}\) by \(O(n^{-1/2})\) and so \(\text{BP}\) is only first-order accurate in general.

For simplifying geometric argument, here we assume \(h_0 = h_1 = 0\) and \(y = (0, \lambda_0)\) by taking the origin of the coordinates at \(\hat{\mu}(H|y)\). Then the signed distance is \(\lambda = \lambda_0\), and the geometric quantities, such as the mean curvature \(\gamma_1\), are now defined at \(\hat{\mu}(H|y) = (0, 0)\). Then the two geometric quantities, \(\lambda_0\) and \(\gamma_1\), determine the \(p\)-value of signed LR = \(\Phi(\lambda_0)\), \(\text{BP} = \Phi(\lambda_0 + \gamma_1) + O(n^{-1})\), and \(\text{PV} = \Phi(\lambda_0 - \gamma_1) + O(n^{-1/2})\) terms. For \(\gamma_1 > 0\), they are ordered as \(\text{BP} < \text{signed LR} < \text{PV}\), and so \(P(\text{BP} < \alpha)\) will be larger than \(P(\text{PV} < \alpha) \approx \alpha\). This confirms (3), where \(\gamma_1\) is defined at \(\mu\) instead of \(\hat{\mu}\) though.

Let us look at the numerical example of \(y = (0.71, 1.63)\) with \(h_0 = 0.1\) in Table 1. We know \(\gamma_1\) is positive by looking at the convex shape of \(H\), and \(\text{BP} = 0.018\) is, in fact, smaller than signed LR = 0.032. From these two values, the mean curvature can be estimated by

\[\gamma_1 = \Phi^{-1}(\text{BP}) - \Phi^{-1}(\text{signed LR}) + O(n^{-1}),\]

which gives \(\gamma_1 \approx 0.018 - 0.032 = 0.028 - 0.53 = 0.23\) at \(\hat{\mu} = (0.12, -0.12)\). We can then compute \(\text{PV}\) up to \(O(n^{-1/2})\) terms as \(\text{PV} \approx \Phi(1.85 - 0.23) = 0.053\), which is close to \(\text{AU3, DBP, and DAU explained in the next sections. On the other hand, the mean curvature} \gamma_1 \approx 0.002\) is much smaller at \(\hat{\mu} = (2.30, -1.33)\) for \(y = (3.18, 0.20)\), and \(\text{PV} \approx 0.038\) is not
different from BP = 0.038; BP does not need bias correction and all the bootstrap methods
are very close to the signed LR in Table 1.

Efron (1985) and Efron and Tibshirani (1998) computed PV up to \(O(n^{-1/2})\) terms in
the same way as above but using only bootstrap probabilities. Their bias-corrected (BC)
bootstrap method estimates the mean curvature by

\[
\gamma_1 = \Phi^{-1} \left( \text{BP}(H|\hat{\mu}(H|y)) \right) + O(n^{-3/2}),
\]

which is verified by letting \(\lambda_0 = 0\) in (11) and (13). In the next sections, we attempt
computing PV up to higher-order terms using only bootstrap probabilities.

3.3. Multiscale bootstrap

For adjusting the bias of BP, we would like to express BP as a function of \(\sigma^2\). Shimodaira
(2002, 2004) showed the asymptotic expansion of BP up to \(O(n^{-1})\) terms. Here we
include \(O(n^{-3/2})\) terms to it. This is an immediate consequence of Theorem 1 via a rescaling
argument.

**Theorem 2** (Scaling-law of the bootstrap probability). For the \(H\) and \(y\) given in Theorem 1,
the bootstrap probability for \(\sigma^2 > 0\) is expressed as

\[
\text{BP}_{\sigma^2}(H|y) = \text{BP}(\sigma^{-1}H|\sigma^{-1}y),
\]

where \(\sigma^{-1}H = \{\sigma^{-1}y : y \in H\}\). By replacing

\[
\beta_0 \rightarrow \sigma^{-1}\beta_0, \quad \beta_1 \rightarrow \sigma\beta_1, \quad \beta_2 \rightarrow \sigma^3\beta_2
\]

in (13), the right hand side of (15) is expressed asymptotically as

\[
\text{BP}_{\sigma^2}(H|y) \approx \Phi \left[ \beta_0\sigma^{-1} + \beta_1\sigma + \beta_2\sigma^3 \right].
\]

Shimodaira (2008) introduced the normalized bootstrap probability defined by

\[
\text{NBP}_{\sigma^2}(H|y) = \Phi \left[ \sigma \Phi^{-1}(\text{BP}_{\sigma^2}(H|y)) \right]
\]

for \(\sigma^2 > 0\), and considered an “approximately unbiased” p-value defined formally by

\[
\text{AU}(H|y) = \text{NBP}_{-1}(H|y).
\]

For extrapolating \(\text{NBP}_{\sigma^2}\) to \(\sigma^2 \leq 0\), we use the scaling-law of BP. It follows from Theorem 2
that the normalized bootstrap probability is expressed asymptotically as

\[
\text{NBP}_{\sigma^2}(H|y) \approx \Phi \left[ \beta_0 + \beta_1\sigma^2 + \beta_2\sigma^4 \right]
\]

for \(\sigma^2 > 0\), and it is extrapolated to \(\sigma^2 \leq 0\) by the right-hand side of (18). In particular for
\(\sigma^2 = -1\), we obtain the asymptotic expansion of AU as

\[
\text{AU}(H|y) \approx \Phi(\beta_0 - \beta_1 + \beta_2).
\]

Comparing (19) with (14), we find that \(\text{AU}(H|y) = \text{PV}(H|y) + O(n^{-3/2})\), indicating AU
is third-order accurate in general. The remaining bias of order \(O(n^{-3/2})\) comes from the
difference \(\Phi^{-1}(\text{AU}) - \Phi^{-1}(\text{PV}) \approx \frac{4}{\gamma_3}\).
In complicated applications, we do not know the values of the coefficients $\beta_0, \beta_1, \beta_2$, or they are just hardly obtained through mathematical analysis. In the multiscale bootstrap of Shimodaira (2008), we estimate $\beta_0, \beta_1, \beta_2$ by fitting the right-hand side of (17) to observed values of $BP_{\sigma^2}(H|y)$ computed for several $\sigma^2 > 0$ values, say, $\sigma^2_1, \ldots, \sigma^2_S$. This is equivalent to fitting quadratic model $\beta_0 + \beta_1 \sigma^2 + \beta_2 (\sigma^2)^2$ in terms of $\sigma^2$ to observed values of $\sigma \Phi^{-1}(BP_{\sigma^2}(H|y))$. Using the estimated values of the coefficients, we can compute (18) for $\sigma^2 \leq 0$. In the original form of multiscale bootstrap of Shimodaira (2002), only two coefficients $\beta_0, \beta_1$ are estimated by linear model $\beta_0 + \beta_1 \sigma^2$, and $p$-value is computed as $AU = \Phi(\beta_0 - \beta_1)$. The difference of the two AU values is only $O(n^{-3/2})$ and both the AU values are third-order accurate.

The procedure is illustrated in Fig 2 for the numerical example of $y = (0.71, 1.63)$ with $h_0 = 0$, where the geometric quantities are actually not defined at the vertex $\mu = (0, 0)$. We plotted $\sigma \Phi^{-1}(BP_{\sigma^2}(H|y))$ in a solid curve for $0.1 < \sigma^2 < 1.9$, instead of plotting the values for $\sigma^2_1, \ldots, \sigma^2_S$. We denote $AU_k$ when extrapolation to $\sigma^2 \leq 0$ is made by Taylor expansion with $k$ terms at $\sigma^2 = 1$. This computes $AU_2 = \Phi(1.69) = 0.046$ by the linear model, and $AU_3 = \Phi(1.53) = 0.062$ by the quadratic model. Interestingly, the procedure behaves similarly to the case of $h_0 = 0.1$, and it seems working fine even when $h_0 = 0$ as will be seen also in the simulation study of Section 3.5.

![Fig 2. Illustration of multiscale bootstrap and multiscale-double bootstrap for $y = (0.71, 1.63)$. The boundary surface $\partial H$ is defined by (5) with $h_0 = 0$. Vertical axis indicates $z = \Phi^{-1}(p)$ for several $p$-values. In multiscale bootstrap, $z = \sigma \Phi^{-1}(BP_{\sigma^2}(H|y))$ is extrapolated to $\sigma^2 = -1$ by linear model (dashed line) or quadratic model (dotted curve). In multiscale-double bootstrap, $z = \Phi^{-1}(DBP_{\sigma^2}(H|y))$ is extrapolated to $\sigma^2 = -1$ by linear model (dashed line).](image)

### 3.4. Multiscale-double bootstrap

The bias of BP can also be adjusted by the iterated bootstrap. Instead of (2), we generate many bootstrap replicates around $\hat{\mu}(H|y)$ by

$$Y^+ \sim N_{q+1}(\hat{\mu}(H|y), \tau^2 I_{q+1})$$

for some $\tau^2 > 0$. The notation $Y^+$ is used to make the distinction clear. For each generated value of $y^+$, we compute $BP_{\sigma^2}(H|y^+)$. This involves second-level bootstrap and huge computation. We calibrate $BP_{\sigma^2}(H|y)$ by the distribution of $BP_{\sigma^2}(H|Y^+)$. The double bootstrap
probability of \( H \) for a given \( y \) is defined as

\[
\text{DBP}_{\tau, \sigma^2}(H|y) = P_{\sigma^2}[\text{BP}_{\sigma^2}(H|Y^+) \leq \text{BP}_{\sigma^2}(H|y) | \hat{\mu}(H|y)].
\]  
(20)

The variances are usually \( \sigma^2 = \tau^2 = 1 \) and we simply denote DBP or DBP(\( H|y \)) for DBP(\( H|y \)). Efron and Tibshirani (1998) called DBP as a calibrated confidence level and mentioned that DBP is third-order accurate.

We will show later in Section 5.3 that the double bootstrap probability for \( \sigma^2 > 0, \tau^2 = 1 \) is expressed asymptotically as

\[
\text{DBP}_{1, \sigma^2}(H|y) \simeq \Phi\left[\beta_0 - \beta_1 - \beta_2 - \beta_3 \sigma^2\right],
\]  
(21)

and it is extrapolated to \( \sigma^2 \leq 0 \) by the right-hand side. Comparing (21) with (14), we find that \( \text{DBP}_{1, \sigma^2}(H|y) = \text{PV}(H|y) + O(n^{-3/2}) \). In particular for \( \sigma^2 = 1 \), we confirm that DBP is third-order accurate.

The remaining bias of order \( O(n^{-3/2}) \) in DBP comes from the difference

\[
\Phi^{-1}(\text{DBP}_{1, \sigma^2}) - \Phi^{-1}(\text{PV}) \simeq -(1 + \sigma^2)\beta_3,
\]

which vanishes when \( \sigma^2 = -1 \). The bias-corrected DBP is defined formally by

\[
\text{DAU}(H|y) = \text{DBP}_{1, -1}(H|y)
\]

so that DAU is forth order accurate. Another advantage of DAU over DBP is robustness against computational error of \( \hat{\mu}(H|y) \) as mentioned in Section 5.3. The name of DAU may be understood in the interpretation

\[
\text{DAU}(H|y) \simeq P_{\sigma^2}[\text{AU}(H|Y^+) \leq \text{AU}(H|y) | \hat{\mu}(H|y)],
\]

which immediately follows from (20) by considering the equivalence of contour surfaces of \( \text{BP}_{\sigma^2}(H|y) \) and \( \text{NBP}_{\sigma^2}(H|y) \) as mentioned just before Lemma 5 in Section 5.1.

Similarly to the computation of AU, we estimate the coefficients \( \beta_0 - \beta_1 - \beta_2 \) and \( \beta_3 \) by fitting a linear model to observed values of \( \Phi^{-1}(\text{DBP}_{1, \sigma^2}) \). The procedure is illustrated in Fig 2. We plotted \( \Phi^{-1}(\text{DBP}_{1, \sigma^2}) \) in a solid curve for \( 0.1 < \sigma^2 < 1.9 \) and extrapolation to \( \sigma^2 = -1 \) is made by Taylor expansion at \( \sigma^2 = 1 \). DAU = \( \Phi(1.48) = 0.069 \) is slightly larger than DBP = \( \Phi(1.54) = 0.061 \) in this example.

### 3.5. Simulation study

Rejection probabilities (3), (4), and those for other approximate \( p \)-values are shown in Table 2. The region \( H \) is the cone-shaped region mentioned in Section 2, where \( h \) is specified by (5) with \( b_0 = 0 \). Rejection probabilities are computed for several \( \mu = (u, -h(u)) \) on \( \partial H \). These values are computed accurately by numerical integration instead of Monte-Carlo simulation for avoiding sampling error. Looking at the table, we verify that MCB is unbiased at \( u = 0 \). However, the rejection probability of MCB is much smaller than \( \alpha \) for larger \( u \).

All the bootstrap methods behave similarly in the sense that the bias is large at \( u = 0 \) and the bias decreases as \( u \) becomes larger. BP has the largest bias, and all the bias-corrected bootstrap probabilities have smaller bias. In particular, AU3, DBP, and DAU have very small bias. The difference between DBP and DAU is small, but DAU performs better than DBP at all \( u \) values. Interestingly, the bias correction methods work fine, even though \( h(u) \) is not smooth at \( u = 0 \). Looking at Table 1 again, we confirm that AU3, DBP, DAU values are close to MCB for \( y = (0.71, 1.63) \), agreeing with the simulation at \( u = 0 \).
4. Geometry of smooth surfaces

In this section, we discuss only geometry of smooth surfaces via simple but tedious calculation without any probability argument. The results will be used in Section 5 for deriving asymptotic accuracy of the bootstrap methods. We work on the region \( H = \mathcal{R}(h) \) and boundary surface \( \partial H = \mathcal{B}(h) \) for \( h \in \mathcal{S} \) expressed in the \((u, v)\) coordinates.

4.1. Representing surfaces in local coordinates

We consider local coordinates \((\Delta u, \Delta v)\) with \( \Delta u = (\Delta u_1, \ldots, \Delta u_q) \in \mathbb{R}^q \) and \( \Delta v \in \mathbb{R} \) by taking the origin at \((u, -h(u))\). A point \((\Delta u, \Delta v)\) is expressed in the \((u, v)\) coordinates as

\[
(u, -h(u)) + \Delta u_i b_i + \Delta v \|f\|^{-1} f
\]

using basis \(\{b_1, \ldots, b_q, f\}\) in \(\mathbb{R}^{q+1}\) defined as follows.

Here \(\|f\| = \sqrt{\int f^2} \) is the norm of \(f \in \mathbb{R}^{q+1}\) with the inner product \(a \cdot b = \sum_{i=1}^{q+1} a_i b_i\) for two vectors \(a, b \in \mathbb{R}^{q+1}\). We denote \(\delta_i = (\delta_{i1}, \ldots, \delta_{iq}) \in \mathbb{R}^q\) with the Kronecker delta \(\delta_{ij}\), and \(\nabla = (\partial/\partial u_1, \ldots, \partial/\partial u_q)\). Then

\[
b_i = \left(\delta_i - \frac{\partial h}{\partial u_i}\right), i = 1, \ldots, q,
\]

are tangent to \(\partial H\) at \((u, -h(u))\), and the normal vector

\[
f = (\nabla h, 1)
\]

satisfies \(f \cdot b_i = 0\), meaning that \(f\) is orthogonal to \(\partial H\) at \((u, -h(u))\). The vectors \(b_i\) and \(f\) should be denoted as \(b_i(u)\) and \(f(u)\), but the dependence on \(u\) is suppressed in the notation.

**Lemma 1.** For \(h \in \mathcal{S}\), the region \(H = \mathcal{R}(h)\) is expressed in the \((\Delta u, \Delta v)\) coordinates at \((u, -h(u))\) as

\[
H = \{ (\Delta u, \Delta v) \mid \Delta v \leq -\tilde{h}(\Delta u), \Delta u \in \mathbb{R}^q \}
\]

with \(\tilde{h} \in \mathcal{S}\). The coefficients are \(\tilde{h}_0 = \tilde{h}_i = 0, \tilde{h}_{ij} = h_{ij} + 3h_{ijk}u_k + (6h_{ijkl} - 2h_{ijk}h_{ml})u_ku_l, \tilde{h}_{ijkl} = h_{ijkl} + 4h_{ijkl}u_l - \frac{1}{4}(h_{ijkm}h_{ml} + h_{ikhm}h_{ml} + h_{jkhm}h_{ml})u_l, \tilde{h}_{ijkl} = h_{ijkl}\).

4.2. Expressions of the four geometric quantities

We consider an orthonormal basis \(\{e_1, \ldots, e_q, \|f\|^{-1} f\}\) for the local coordinates at \((u, -h(u))\), where \(\{e_1, \ldots, e_q\}\) is an arbitrary orthonormal basis of the tangent space; \(e_i \cdot e_j = \delta_{ij}\) and \(e_i \cdot f = 0\). The dependence of these vectors on \(u\) is suppressed in the notation again. A point \((x, \Delta v)\) with \(x = (x_1, \ldots, x_q) \in \mathbb{R}^q\) and \(\Delta v \in \mathbb{R}\) corresponds to

\[
(u, -h(u)) + \Delta u_i e_i + \Delta v \|f\|^{-1} f
\]
in the \((u, v)\) coordinates.

In the \((x, \Delta v)\) coordinates, \(\partial H\) is expressed as \(\Delta v = -d(x)\) with

\[
d(x) \simeq d_{ij}x_i x_j + d_{ijk}x_i x_j x_k + d_{ijkl}x_i x_j x_k x_l.
\]

Then we apply the definitions of \(\gamma_i\) in (10) to \(d(x)\) as follows.

\[
\begin{align*}
\gamma_1(h, u) &= d_{ii} = \text{tr}(D), \\
\gamma_2(h, u) &= d_{ij}d_{ij} = \text{tr}(D^2), \\
\gamma_3(h, u) &= d_{ij}d_{jk}d_{kl} = \text{tr}(D^3), \\
\gamma_4(h, u) &= d_{ijkl}.
\end{align*}
\]

where \(D\) is \(q \times q\) matrix with elements \((D)_{ij} = d_{ij}\). The four geometric quantities are invariant to the choice of orthonormal basis as will be seen in (23) below.

**Lemma 2.** For \(h \in S\), we consider the local coordinates \((\Delta u, \Delta v)\) at \((u, -h(u))\) using the basis \(\{b_1, \ldots, b_q, f\}\). Let \(G\) be \(q \times q\) matrix with elements \((G)_{ij} = g_{ij} = b_i \cdot b_j\) for \(i, j = 1, \ldots, q\), and \(g^{ij} = (G^{-1})_{ij}\) be the elements of the inverse matrix of \(G\). Then the four geometric quantities are expressed as

\[
\begin{align*}
\gamma_1(h, u) &= \tilde{h}_{ij}g^{ij} = \text{tr}(\tilde{D}G^{-1}), \\
\gamma_2(h, u) &= \tilde{h}_{ij}g^{ij}h_{ij}g^{ij} = \text{tr}((\tilde{D}G^{-1})^2), \\
\gamma_3(h, u) &= \tilde{h}_{ij}g^{ij}h_{kl}g^{lm}h_{mn}g^{ni} = \text{tr}((\tilde{D}G^{-1})^3), \\
\gamma_4(h, u) &= \tilde{h}_{ijkl}g^{ij}g^{kl},
\end{align*}
\]

using the coefficients \(\tilde{h}_{ij}\) and \(\tilde{h}_{ijkl}\) defined in Lemma 1 and \(q \times q\) matrix \(\tilde{D}\) with elements \((\tilde{D})_{ij} = \tilde{h}_{ij}\). They are expressed asymptotically as

\[
\begin{align*}
\gamma_1(h, u) &\simeq h_{ii} + 3h_{iik}u_k + (6h_{ikl} - 2h_{iik}h_{km}h_{ml} - 4h_{ij}h_{ik}h_{ji}u_ku_l), \\
\gamma_2(h, u) &\simeq h_{ij}h_{ij} + 6h_{ij}h_{jkl}u_k, \\
\gamma_3(h, u) &\simeq h_{ij}h_{jkl}, \\
\gamma_4(u, h) &\simeq h_{ij}
\end{align*}
\]

using the coefficients of \(h(u)\). In particular, \(\gamma_i = \gamma_i(h, 0), i = 1, \ldots, 4\), are consistent with their definitions in (10). Also,

\[
\begin{align*}
\frac{1}{2} \frac{\partial^2 \gamma_1(h, u)}{\partial u_i \partial u_j} &\bigg|_0 \simeq 6h_{mni}u_i - 2h_{mm}h_{ii}u_j - 4h_{mi}h_{mi}u_{ij}
\end{align*}
\]

confirms that the definition of \(\beta_3\) in (11) is consistent with (8).

**4.3. Shifting surfaces**

We consider shifting \(B(h)\) toward the normal direction. Let \(f(u)\) be the normal vector at \((u, -h(u)) \in B(h)\). For a specified \(\lambda \in S\), we move the point \((u, -h(u))\) by \(\lambda(u)\) toward the normal direction. This is expressed as

\[
(\theta, -s(\theta)) = (u, -h(u)) + \lambda(u)||f(u)||^{-1}f(u),
\]

where \(s(u)\) is some function of \(u \in \mathbb{R}^q\), and \(\theta \in \mathbb{R}^q\) is used when distinction is needed. We can interpret (25) as

\[
\tilde{\mu}(H|((\theta, -s(\theta)))) = (u, -h(u))
\]

with signed distance \(\lambda(u)\). For sufficiently large \(n\), such \(s(\theta)\) is uniquely defined for each \(\theta\), because all the surfaces approach flat as \(n \to \infty\). We denote (25) as

\[
s = \mathcal{M}(h, \lambda).
\]
Lemma 3. Let $s = \mathcal{M}(h, \lambda)$ for $h \in \mathcal{S}$, $\lambda \in \mathcal{S}$. If $\lambda(u)$ is expressed as

$$\lambda(u) \simeq \lambda_0 + \lambda_i u_i + \lambda_{ij} u_i u_j$$

with $\lambda_0 = O(1)$, $\lambda_i = O(n^{-1})$, $\lambda_{ij} = O(n^{-3/2})$, then we have $s \in \mathcal{S}$ with coefficients

$s_0 = h_0 - \lambda_0 = O(1)$, $s_i = h_i - \lambda_i - 2\lambda_0 h_{mi}(h_m - \lambda_m) = O(n^{-1})$, $s_{ij} = h_{ij} - \lambda_{ij} - 2\lambda_0 h_{mj} h_{mi} + 4\lambda_0^2 h_{mi} h_{mj} h_{ij} = O(n^{-1/2})$, $s_{ijk} = h_{ijk} - 2\lambda_0 (h_{mi} h_{mj} + h_{mj} h_{mk} + h_{mk} h_{mi}) = O(n^{-1})$, $s_{ijkl} = h_{ijkl} = O(n^{-3/2})$. The four geometric quantities at $(0, -s(0))$ are $\gamma_1(s, 0) = s_i \simeq \gamma_1 - \lambda_i - 2\lambda_0 \gamma_2 + 4\lambda_0^2 \gamma_3$, $\gamma_2(s, 0) = s_{ij} \simeq \gamma_2 - 4\lambda_0 \gamma_3$, $\gamma_3(s, 0) = s_{ijk} \simeq \gamma_3$, $\gamma_4(s, 0) = s_{ijkl} \simeq \gamma_4$, where $\gamma_i = \gamma_i(h, 0)$, $i = 1, \ldots, 4$.

5. Asymptotic analysis of bootstrap methods

We are going to show the asymptotic expansions of PV and DBP, and then prove the asymptotic accuracy of the bootstrap methods. The argument is based on the geometric tools developed in Section 4 as well as another tool to be developed below.

5.1. Contour surfaces of bootstrap probability

We consider a surface on which the bootstrap probability remains constant. For $H = R(h)$ with $h \in \mathcal{S}$, we consider a function $s(u)$ of $u \in \mathbb{R}^q$ satisfying

$$BP_{\sigma^2}(H|u, -s(u)) = 1 - \alpha, \quad u \in \mathbb{R}^q,$$

meaning $BP_{\sigma^2}(H|y) = 1 - \alpha$ is constant for any $y \in \mathcal{B}(s)$. Then, $\mathcal{B}(s)$, as well as $s$ itself, will be called as the contour surface of the bootstrap probability of $H$ with variance $\sigma^2 > 0$ at level $1 - \alpha$. In particular, we choose $\alpha$ so that $(0, \lambda_0 - h_0) \in \mathcal{B}(s)$ for a specified $\lambda_0 \in \mathbb{R}$. We denote this contour surface as

$s = L_{\sigma^2}(h, \lambda_0)$.

Lemma 4. Let $s = L_{\sigma^2}(h, \lambda_0)$ for $h \in \mathcal{S}$, $\lambda_0 \in \mathbb{R}$, and $\sigma^2 > 0$. Then, $s$ is expressed as $s = \mathcal{M}(h, \lambda)$ by specifying $\lambda(u) \simeq \lambda_0 + \lambda_i u_i + \lambda_{ij} u_i u_j$ with $\lambda_0 = O(1)$,

$$\lambda_i = \sigma^2(-3h_{mi} + 6\lambda_0 h_{mi} h_{ml}), \quad \lambda_{ij} = \sigma^2(-6h_{mij} + 2h_{mmi} h_{lj} + 4h_{mi} h_{mj}). \quad (26)$$

We have $s \in \mathcal{S}$ with coefficients

$s_0 = h_0 - \lambda_0$, $s_i = h_i - 2\lambda_0 h_{mi} + \sigma^2(3h_{mmi} - 6\lambda_0 h_{mi} h_{ml} - 6\lambda_0 h_{mi} h_{ml})$, $s_{ij} = h_{ij} - 2\lambda_0 h_{mi} h_{mj} + 4\lambda_0^2 h_{mi} h_{mj} h_{ij} + \sigma^2(6h_{mmj} - 2h_{mmi} h_{lj} + 4h_{mi} h_{mj})$, $s_{ijkl} = h_{ijkl}$. The four geometric quantities of $s$ at $(0, -s(0))$ are

$$\gamma_1(s, 0) \simeq \gamma_1 - 2\lambda_0 \gamma_2 + 4\lambda_0^2 \gamma_3 + \sigma^2(6\gamma_4 - 2\gamma_1 \gamma_2 - 4\gamma_3), \quad \gamma_2(s, 0) \simeq \gamma_2 - 4\lambda_0 \gamma_3, \quad \gamma_3(s, 0) \simeq \gamma_3, \quad \gamma_4(s, 0) \simeq \gamma_4,$$

where $\gamma_i = \gamma_i(h, 0)$, $i = 1, \ldots, 4$.

We denote the $\lambda(u)$ of (26) as $\lambda_{\sigma^2}(u) = \lambda_0 - \sigma^2 \kappa(u)$ with

$$\kappa(u) = \gamma_1(h, u) - \gamma_1(h, 0) - \lambda_0(\gamma_2(h, u) - \gamma_2(h, 0)) \simeq (3h_{mmi} - 6\lambda_0 h_{mi} h_{ml}) u_i + (6h_{mij} - 2h_{mmi} h_{lj} + 4h_{mi} h_{mj}) u_i u_j. \quad (29)$$
This also relates to (8) as \((1/2)\partial^2 k(u)/\partial u_i \partial u_j = \beta_3\) or \((1/2)\partial^2 \lambda_{\sigma^2}(u)/\partial u_i \partial u_j = -\sigma^2 \beta_3\). The contour surface of \(BP_{\sigma^2}(H|y)\) for \(\sigma^2 > 0\) is expressed asymptotically as

\[ L_{\sigma^2}(h, \lambda_0) = M(h, \lambda_{\sigma^2}), \]

and it is extrapolated formally to \(\sigma^2 \leq 0\) by the right-hand side. It becomes the surface with constant signed distance \(\lambda(u) = \lambda_0\) when \(\sigma^2 = 0\). For \(\sigma^2 \in \mathbb{R}\), the deviation \(\lambda_{\sigma^2}(u) - \lambda_0 = -\sigma^2 k(u)\) is proportional to \(\sigma^2\). Therefore, the formal definition of \(L_{\sigma^2}(h, \lambda_0)\) for \(\sigma^2 < 0\) makes sense, at least, in terms of computation, although \(BP_{\sigma^2}(H|y)\) is not defined. In fact, \(L_{\sigma^2}(h, \lambda_0)\) is interpreted as the contour surface of \(NBP_{\sigma^2}(H|y)\) for \(\sigma^2 \in \mathbb{R}\), because we will get the same expression of \(\lambda_{\sigma^2}(u)\) for \(NBP_{\sigma^2}(H|y) = 1 - \alpha'\) by substituting \(\sigma z_\alpha = z_{\alpha'}\) in the proof of Lemma 4.

**Lemma 5.** Two functions \(h, s \in S\) are denoted as \(h \overset{\dagger}{=} s\), if \(h_0 = s_0, h_{ij} = s_{ij}, h_{ijk} = s_{ijk}\), and \(h_{ijkl} = s_{ijkl}\) by ignoring the difference between \(h_i\) and \(s_i\). Then, for \(\lambda_0, \xi_0, \sigma^2, \tau^2 \in \mathbb{R}\), the following additivity property holds:

\[ L_{\sigma^2}(L_{\sigma^2}(h, \lambda_0), \xi_0) = L_{\sigma^2 + \tau^2}(h, \lambda_0 + \xi_0). \]  

(30)

As a special case, “\(\overset{\dagger}{=}\)” in (30) is replaced by “\(\sim\)” if \(\sigma^2 \xi_0 = \tau^2 \lambda_0\). In particular, the identity operator \(L_0(h, 0) \simeq h\), and the inverse operator

\[ L_{-\sigma^2}(L_{\sigma^2}(h, \lambda_0), -\lambda_0) \simeq h \]

hold for the \(h_i\) term too.

### 5.2. Asymptotic expansion of the unbiased p-value

We are now prepared to derive the expression of the fourth-order accurate p-value mentioned in Section 3.2. We consider a surface on which PV remains constant. For \(H = R(h)\) with \(h \in S\), we consider a function \(s(u)\) of \(u \in \mathbb{R}^q\) satisfying

\[ PV(H|u, -s(u)) = \alpha, \quad u \in \mathbb{R}^q, \]

meaning \(PV(H|y) = \alpha\) is constant for any \(y \in B(s)\). For a specified significance level \(\alpha\), we will reject \(H_0\) if \(y \not\in R(s)\), and accept \(H_0\) if \(y \in R(s)\). Since PV is fourth-order accurate, the acceptance probability for any \(\mu = (\theta, -h(\theta)) \in \partial H\) is expressed as

\[ BP(R(s)|(\theta, -h(\theta))) \simeq 1 - \alpha, \quad \theta \in \mathbb{R}^q, \]

meaning \(\partial H\) is the contour surface of the bootstrap probability of \(R(s)\).

For a specified \(y = (0, \lambda_0 - h_0)\), we will choose the value of \(\alpha\) so that \(y \in B(s)\). Considering \((0, \lambda_0 - h_0) \in B(s) \Leftrightarrow \lambda_0 - h_0 = -s_0 \Leftrightarrow (0, -\lambda_0 - s_0) \in \partial H\), we have

\[ h \simeq L_1(s, -\lambda_0). \]

Using the inverse operator in Lemma 5, the contour surface of PV is expressed as

\[ s \simeq L_{-1}(h, \lambda_0). \]

The expression of \(PV(H|y)\) will be obtained as \(\alpha\) for \(y \in B(s)\), and thus, by choosing \(\mu = (0, -h_0)\) with \(\theta = 0\), we get

\[ PV(H|y) \simeq 1 - BP(R(s)|(0, -h_0)). \]
For applying Theorem 1 to $BP(R(s)|(0,-h_0))$, we would like to replace $h \to s$ and $\lambda_0 - h_0 \to -s$ in $BP(R(h)|(0,\lambda_0 - h_0))$. This implies replacing $\lambda_0 \to -\lambda_0$ as well as $\gamma_i \to \gamma_i(s,0)$ in (12), because $\lambda_0 - h_0 \to (-\lambda_0) - s_0 = -h_0$ as desired. This is equivalent to replacing $\beta_0 \to -\beta_0$, $\beta_1 \to -\beta_1$, $\beta_2 \to \beta_2$ in (13) as shown in the proof of the theorem below, and therefore, we obtain $PV(H|y) \simeq 1 - \hat{\Phi}((\beta_0 + (\beta_1 - \beta_3) + \beta_2) = \hat{\Phi}(\beta_0 - \beta_1 - \beta_2 + \beta_3).

Theorem 3 (Fourth-order accurate p-value). For the $H$ and $y = (0,\lambda_0 - h_0)$ given in Theorem 1, an approximately unbiased p-value of fourth-order accuracy is expressed asymptotically as (14).

Related results are given in Theorem 1 of Shimodaira (2008), from which we borrowed the idea of the inverse operator. An unusual asymptotic theory of “nearly flat” surfaces is discussed there by utilizing Fourier transform of surfaces instead of Taylor series for handling non-smooth surfaces such as cones.

5.3. Asymptotic expansion of the double bootstrap probability

To see the robustness of DBP against computational error in the minimization of (6), we replace $\hat{\mu}(H|y)$ in (20) by $\hat{\mu} = (\theta, -h(\theta)) \in \partial H$ for some $\theta \in \mathbb{R}$. We assume $\theta = O(1)$, meaning that the computational error is $O(n^{-1/2})$ with respect to the original parameter, say, $\eta$ in the spherical example. We denote $DBP_{\tau, \sigma^2}(H|y)$ for this modified double bootstrap probability, and derive its asymptotic expansion for $y = (0,\lambda_0 - h_0)$.

First note that $BP_{\tau, \sigma^2}(H|Y^+) \geq BP_{\sigma^2}(H|y) \Rightarrow Y^+ \in R(s)$ for $s = L_{\sigma^2}(h, \lambda_0)$, and

$$DBP_{\tau, \sigma^2}(H|y) = 1 - BP_{\tau, \sigma^2}(R(s)|\hat{\mu}).$$

By applying Theorem 2 to $BP_{\tau, \sigma^2}(R(s)|\hat{\mu})$, we get the following theorem via a straightforward computation.

Theorem 4 (Scaling-law of the double bootstrap probability). For the $H$ and $y = (0,\lambda_0 - h_0)$ given in Theorem 1, the modified double bootstrap probability with $\hat{\mu} = (\theta, -h(\theta))$ is expressed asymptotically as

$$DBP_{\tau, \sigma^2}(H|y) \simeq \hat{\Phi}\left[\beta_0 \tau^{-1} - \beta_1 \tau - \beta_2 \tau^3 - \beta_3 \tau \sigma^2 - \tau^{-1}(\tau^2 + \sigma^2)\kappa(\theta)\right],$$

where $\kappa(\theta)$ is defined in (29).

When $h_i = 0$, we have $\hat{\mu}(H|y) = (0,-h_0)$. By letting $\theta = 0$ in (31), we obtain

$$DBP_{\tau, \sigma^2}(H|y) \simeq \hat{\Phi}\left[\beta_0 \tau^{-1} - \beta_1 \tau - \beta_2 \tau^3 - \beta_3 \tau \sigma^2\right].$$

When $h_i = O(n^{-1})$, we have $\hat{\mu}(H|y) = (\theta, -h(\theta))$ with some $\theta = O(n^{-1})$ for which $\kappa(\theta) \simeq 0$. Therefore, (32) holds for any $h \in S$, and (21) follows. This argument also confirms that the four geometric quantities as well as $\beta_i$ defined at $\theta = 0$ are interpreted as those defined at $\mu(H|y)$, because $\gamma_i(h,\theta) \simeq \gamma_i$ for $\theta = O(n^{-1})$.

Comparing (31) with (32), we find that $\kappa(\theta)$ represents deviation of $DBP_{\tau, \sigma^2}(H|y)$ from $DBP_{\tau, \sigma^2}(H|y)$ due to computational error of $\hat{\mu}(H|y)$. For $\theta = O(1)$, the deviation is $\kappa(\theta) = O(n^{-1})$. $DBP_{1,1}(H|y) = DBP_{1,1}(H|y) + O(n^{-1})$ and thus DBP is degraded from third-order accurate to second-order accurate under the computational error. However, the deviation disappears in (31) when $\sigma^2 = -\tau^2$. In particular, $DBP_{1,1}(H|y) \simeq DBP_{1,1}(H|y)$ and thus DAU remains fourth-order accurate even if there is computational error of $\theta = O(1)$. 


Let us assume that $\partial H$ is a constant-mean-curvature surface. Noting $\gamma_1(h, \theta) = \gamma_1$ for any $\theta = O(1)$, we have $h_{mm} = 0$, $6h_{mm}h_{ij}h_{ij} - 2h_{mm}h_{mi}h_{mj} = 0$, and thus $\kappa(\theta) = -6\lambda_{m}h_{mm}h_{mi}h_{mj} = O(n^{-3/2})$. Therefore, DBP is degraded from fourth-order accurate to third-order accurate. In addition, we may assume that $\gamma_2(h, \theta) = \gamma_2$ for any $\theta = O(1)$, and so $h_{mm}h_{mi} = 0$; this is the case for the spherical example. Then the deviation $\kappa(\theta) \approx 0$, and DBP remains fourth-order accurate. Therefore, DBP is as good as DAU under these conditions.

5.4. Asymptotic accuracy of bootstrap methods

For deriving the rejection probabilities (3) and (4) mentioned in Section 1, here we assume that $\mu = (0, -h_0)$ in the $(u, v)$ coordinates. Thus the expressions of $\gamma_i$ and $\beta_i$ in Section 3.1 are now interpreted as geometric quantities defined at $\mu \in \partial H$ instead of $\hat{\mu}(H|y)$.

First we consider testing $H_0$ by using $\text{NBP}_{\alpha^2}(H|y)$ as an approximate $p$-value. For a given $\alpha$, we may choose $\lambda_0 \in \mathbb{R}$ so that $\text{NBP}_{\alpha^2}(H|(0, \lambda_0 - h_0)) = \alpha$. Then the acceptance region is expressed as $\{y|\text{NBP}_{\alpha^2}(H|y) \geq \alpha\} = \mathcal{R}(s)$ using $s = \mathcal{L}_{\alpha^2}(h, \lambda_0)$, and thus

$$P\left(\text{NBP}_{\alpha^2}(H|Y) < \alpha\right) = 1 - \text{BP}(\mathcal{R}(s)|(0, -h_0)).$$

This is computed as $\text{DBP}_{1, \alpha^2}(H|(0, \lambda_0 - h_0))$ with $\tilde{\mu} = (0, -h_0)$ in the theorem below.

**Theorem 5** (Rejection probability of the normalized bootstrap probability). For the $H$ given in Theorem 1, and $\mu = (0, -h_0) \in \partial H$, the rejection probability of $\text{NBP}_{\alpha^2}(H|y)$ is

$$P\left(\text{NBP}_{\alpha^2}(H|Y) < \alpha\right) \simeq \Phi\left[z_{\alpha} + (1 + \sigma^2)\left\{\gamma_1 + z_{\alpha}\gamma_2 + \frac{4}{3}z_{\alpha}\gamma_3 - \gamma_1\gamma_2\right\} + (1 + \sigma^2)^2\left\{3\gamma_4 - \frac{4}{3}\gamma_3\right\} - \sigma^2\frac{4}{3}\gamma_3\right].$$

(33)

In particular, $\sigma^2 = 1$ gives (3), and $\sigma^2 = -1$ gives

$$P\left(\text{AU}(H|Y) < \alpha\right) \simeq \Phi(z_{\alpha} + \frac{4}{3}\gamma_3) = \alpha + O(n^{-3/2}).$$

Therefore BP is first-order accurate, and AU is third-order accurate.

Next we consider testing $H_0$ by using $\text{DBP}_{1, \alpha^2}(H|y)$ as an approximate $p$-value. For a given $\alpha$, we may choose $\lambda_0 \in \mathbb{R}$ so that $\text{DBP}_{1, \alpha^2}(H|(0, \lambda_0 - h_0)) = \alpha$. We will see, in the proof of the theorem below, the acceptance region is expressed as $\{y|\text{DBP}_{1, \alpha^2}(H|y) \geq \alpha\} = \mathcal{R}(s)$ using $s = \mathcal{L}_{-1}(h, \lambda_0)$, and thus the rejection probability is $1 - \text{BP}(\mathcal{R}(s)|(0, -h_0))$. This is computed as $\text{DBP}_{1, -1}(H|(0, \lambda_0 - h_0))$ with $\tilde{\mu} = (0, -h_0)$.

**Theorem 6** (Rejection probability of the double bootstrap probability). For the $H$ given in Theorem 1, and $\mu = (0, -h_0) \in \partial H$, the rejection probability of $\text{DBP}_{1, \alpha^2}(H|y)$ is

$$P\left(\text{DBP}_{1, \alpha^2}(H|Y) < \alpha\right) \simeq \Phi\left[z_{\alpha} - (1 + \sigma^2)\beta_3\right].$$

(34)

In particular, $\sigma^2 = 1$ gives (4), and $\sigma^2 = -1$ gives

$$P\left(\text{DAU}(H|Y) < \alpha\right) \simeq \alpha.$$

Therefore, DBP is third-order accurate, and DAU is fourth-order accurate.
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Appendix

The following lemma is used in the proof of Theorem 1 below.

Lemma 6 (Moments of normal random variables). Let \( \delta_{ij} \) denote the Kronecker delta, and indices \( i, j, \ldots \in \{1, \ldots, q\} \). Consider the multivariate normal distribution \( (U_1, \ldots, U_q) \sim N_q(0, I_q) \). Then the first three even-order moments are

\[
E(U_i U_j) = \delta_{ij}, \quad E(U_i U_j U_k U_l) = \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk},
\]

\[
E(U_i U_j U_k U_l U_m U_n) = \delta_{ij} \delta_{kl} \delta_{mn} + \delta_{ik} \delta_{jl} \delta_{mn} + \cdots + \delta_{in} \delta_{jk} \delta_{lm}.
\]

For \( k = 1, 2, \ldots \), the expectation of the product of \( 2k \) variables \( E(U_{i_1} \cdots U_{i_{2k}}) \) is the sum of \( (2k)!/(2^k k!) \) terms of partitioning \( \{i_1, \ldots, i_{2k}\} \) into \( k \) pairs, where each term is the product of \( k \) Kronecker deltas corresponding to the \( k \) pairs. On the other hand, odd-order moments are all zero;

\[
E(U_i) = E(U_i U_j U_k) = E(U_i U_j U_k U_l U_m) = \cdots = 0.
\]

Proof of Lemma 6. This lemma is a direct consequence of the general result of Isserlis (1918) for \( U \sim N_q(0, \Sigma) \) with any covariance \( \Sigma \).

Proof of Theorem 1. We denote \( Y^* = (U, V) \) in the \( (u, v) \) coordinates so that (2) is expressed as

\[
U \sim N_q(0, \sigma^2 I_q), \quad V \sim N(\lambda_0 - h_0, \sigma^2).
\]

The bootstrap probability for \( \sigma^2 = 1 \) is expressed as \( P((U, V) \in H) = P(V \leq -h(U)) = E \left[ P(V \leq -h(U)|U) \right] = E \left[ \Phi(-\lambda_0 + h(U)) \right] \). For calculating the term in the brackets, we consider the Taylor series

\[
\Phi(-a - x) = \Phi(-a) + n(a) \left[ -x + \frac{1}{2} ax^2 + \frac{1}{6} (1 - a^2)x^3 \right] + O(x^4),
\]

with \( a = \lambda_0 \) and \( x = h(U) - h_0 \simeq h_{ii} U_i + h_{ij} U_j + h_{ik} U_i U_k + h_{ijkl} U_i U_j U_k U_l \). Then we have

\[
P((U, V) \in H) \simeq \Phi(-a) + n(a) \left[ -E(x) + \frac{1}{2} aE(x^2) + \frac{1}{6} (1 - a^2)E(x^3) \right].
\]

For calculating \( E(x) \), \( E(x^2) \), and \( E(x^3) \), we use Lemma 6. By noticing (9), \( E(x) \simeq h_{ij} E(U_i U_j) + h_{ijkl} E(U_i U_j U_k U_l) \), and \( E(x^2) \simeq h_{ij} h_{kl} E(U_i U_j U_k U_l) \), and \( E(x^3) \simeq h_{ijkl} h_{km} E(U_i U_j U_k U_l U_m U_n) \), we have

\[
P((U, V) \in H) \simeq \Phi(a) - \frac{1}{2} a(\gamma_1 + 3\gamma_4) + \frac{1}{6} a^2 (\gamma_1^3 + 6\gamma_1 \gamma_2 + 8\gamma_3) + O(n^{-2}).
\]

Substituting these moments in (36), we have

\[
P((U, V) \in H) \simeq \Phi(-a - x) = \Phi(a + x),
\]

and we get (12).
Proof of Theorem 2. Considering $Y^* \in H \iff \sigma^{-1} Y^* \in \sigma^{-1} H$, we have $B_{\sigma}(H|y) = P_{\sigma}(Y^* \in H|y) = P_{\sigma}(\sigma^{-1} Y^* \in \sigma^{-1} H|y) = B_{\sigma}(\sigma^{-1} H|\sigma^{-1} y)$, where the last equation follows from $\sigma^{-1} Y^* \sim N_{n+1}(\sigma^{-1} y, I_{n+1})$. This proves (15). We only have to show that replacing $H \rightarrow \sigma^{-1} H$ and $y \rightarrow \sigma^{-1} y$ in (13) implies (16). In the $(u, v)$ coordinates, the $k$-th derivative $\partial^k h(u)/\partial u_i \cdots \partial u_k$ is multiplied by $\sigma^{k-1}$, because all the terms in the numerator and the denominator are scaled by $\sigma^{-1}$. Thus $H \rightarrow \sigma^{-1} H$ is expressed as $h_0 \rightarrow \sigma^{-1} h_0, h_1 \rightarrow h_1, h_{ij} \rightarrow \sigma h_{ij}, h_{ijkl} \rightarrow \sigma^2 h_{ijkl}, h_{ijklm} \rightarrow \sigma^3 h_{ijklm}$, and then $\gamma_1 \rightarrow \sigma \gamma_1, \gamma_2 \rightarrow \sigma^2 \gamma_2, \gamma_3 \rightarrow \sigma^3 \gamma_3, \gamma_4 \rightarrow \sigma^3 \gamma_4$. $y \rightarrow \sigma^{-1} y$ is expressed as $\lambda_0 \rightarrow \sigma^{-1} \lambda_0$. Applying these rules to (11), we get (16). \hfill \box

Proof of Lemma 1. A point $(\Delta u, -\hat{h}(\Delta u))$ on $\partial H$ in the $(\Delta u, \Delta v)$ coordinates is expressed as $(u + \Delta u, -h(u + \Delta u))$ in the $(u, \Delta v)$ coordinates for some $\Delta \tilde{u} = (\Delta \tilde{u}_i, \Delta \tilde{u}_j) \in \mathbb{R}^q$. Substituting $\Delta v = -\hat{h}(\Delta u)$ in (22), we have $(u + \Delta \tilde{u}, -h(u + \Delta \tilde{u})) = (u, -h(u)) + \Delta u b_i - \hat{h}(\Delta u)\|f\|^{-1} f$, and thus, using the definitions of $b_i$ and $f$, we get
\[
\Delta \tilde{u}_i = \Delta u_i - \hat{h}(\Delta u)\|f\|^{-1} \frac{\partial h}{\partial u_i}, \quad i = 1, \ldots, q, \tag{38}
\]
\[
h(u + \Delta \tilde{u}) = h(u) + \Delta u i \frac{\partial h}{\partial u_i} - \hat{h}(\Delta u)\|f\|^{-1}. \tag{39}
\]
We are going to solve these equations to find the expression of $\hat{h}(\Delta u)$ by eliminating $\Delta \tilde{u}$ from (38) and (39). We first consider the asymptotic order of the terms in (38). $\hat{h}(\Delta u) = O(n^{-1/2})$ because $h(u) = O(n^{-1/2})$ for any $u$. $\|f\| = 1 + O(n^{-1})$ as shown later. $\partial h/\partial u_i = h_i + 2h_{ij}u_j + \cdots = O(n^{-1/2})$. It then follows from (38) that $\Delta \tilde{u}_i - \Delta u_i = O(n^{-1/2} n^{-1/2}) = O(n^{-1})$. We next consider the Taylor expansion of $h(u + \Delta \tilde{u})$ around $u + \Delta u$. $h(u + \Delta \tilde{u}) \approx h(u) + \frac{\partial h}{\partial u_i}|_{u=\Delta \tilde{u}}((\Delta u_i - \Delta u_i) + O(n^{-1/2} \|\Delta \tilde{u} - \Delta u_i\|^2)) \approx h(u + \Delta u) - \frac{\partial h}{\partial u_i}|_{u=\Delta \tilde{u}} \hat{h}(\Delta u)\|f\|^{-1} \frac{\partial h}{\partial u_i}|_{u=\Delta \tilde{u}}$. Substituting this into the left hand side of (39), we solve the equation for $\hat{h}(\Delta u)$. Then we have $\hat{h}(\Delta u) \approx \|f\|AB$ with
\[
A = \left(1 + \frac{\partial h}{\partial u_i}|_{u=\Delta \tilde{u}} \frac{\partial h}{\partial u_i}|_{u=\Delta \tilde{u}} \right)^{-1}, \quad B = h(u + \Delta u) - h(u) - \Delta u \frac{\partial h}{\partial u_i}. \]
We look at the three factors $\|f\|$, $A$, and $B$. The first factor is $\|f\| = \{1 + \sum_{i=1}^{q} (\partial h/\partial u_i)^2\}^{1/2} \approx 1 + (1/2) \sum_{i=1}^{q} (\partial h/\partial u_i)^2$. By noting $\partial h/\partial u_i \approx h_i + 2h_{ij}u_j + 3h_{ijk}u_ju_k + 4h_{ijkl}u_ju_ku_l + 6h_{ijklm}u_ju_ku_lu_m = 1 + 2h_{ij}h_{ik}u_i u_k + O(n^{-3/2})$. The second factor is $A \approx 1 - (\partial h/\partial u_i)|_{u=\Delta \tilde{u}}((\partial h/\partial u_i)|_{u=\Delta \tilde{u}} - \{h_{ij} + 2h_{ij}u_j + O(n^{-1})\}) = 1 - 4h_{ij}h_{ik}u_i u_k + 4h_{ij}h_{ik}u_i u_k + O(n^{-3/2})$. The third factor is $B \approx (1/2)(\partial^2 h/\partial u_i\partial u_j)\Delta u_i \Delta u_j + (1/6)(\partial^3 h/\partial u_i\partial u_j\partial u_k)\Delta u_i \Delta u_j \Delta u_k + (1/24)(\partial^4 h/\partial u_i\partial u_j\partial u_k\partial u_l)\Delta u_i \Delta u_j \Delta u_k \Delta u_l \approx (h_{ij} + 3h_{ijk}u_k + 6h_{ijkl}u_ku_l)\Delta u_i \Delta u_j + (h_{ij} + 3h_{ijk}u_k + 6h_{ijkl}u_ku_l)\Delta u_i \Delta u_j + h_{ijkl}u_i u_j u_k u_l$. Simply multiplying the three factors and collect terms with respect to $\Delta u$, we obtain $\hat{h}(\Delta u) \approx \|f\|AB \approx B + \Delta u_i h_{ij}(2h_{mk}h_{ml}u_k u_l - 4h_{mk}h_{ml}u_k u_l) + \Delta u_i \Delta u_j h_{ij}\{h_{ij} + 3h_{ijk}u_k + 6h_{ijkl}u_ku_l\} + \Delta u_i \Delta u_j \Delta u_k h_{ijk} + \Delta u_i \Delta u_j \Delta u_k h_{ijk} + \Delta u_i \Delta u_j \Delta u_k h_{ijk}$. Looking at the coefficients, we get $h_{ij}$ and $h_{ijk}$. We also get $h_{ijk} = h_{ijk} + 4h_{ijkl} - 4h_{ij}h_{mk}h_{ml}u_i$, which becomes $h_{ijk}$ in the lemma by symmetrization with respect to permutation of indices. \hfill \box

Proof of Lemma 2. Consider a change of coordinates $x \leftrightarrow \Delta u$ in the tangent space as $c_i x_i = b_i \Delta u_i$. Treating $c_i$, $b_i$, $x$, $\Delta u$ as column vectors (although they were defined as row vectors earlier), we write $Cx = B \Delta u$ in the matrix notation using $C = (c_1, \ldots, c_q)$, $B = (b_1, \ldots, b_q)$,
and thus $\Delta u = B^{-1} C x$. Considering $\tilde{h}(\Delta u) = d(x)$ for any $x$, we have $\tilde{h}_{ij} \Delta u_i \Delta u_j = d_{ij} x_i x_j$, $\tilde{h}_{ijk} \Delta u_i \Delta u_j \Delta u_k = d_{ijk} x_i x_j x_k$, etc. Substituting $\Delta u = B^{-1} C x$ in $\Delta u^T D \Delta u = x^T D x$, we have $D = C^T (B^{-1})^T D B^{-1} C$, where $T$ denotes matrix transpose. Noting $C^T C = CC^T = I$ and $B^T B = G$, we obtain $\text{tr}(D) = \text{tr}(C^T (B^{-1})^T D B^{-1} C) = \text{tr}(C^T (B^{-1})^T) = \text{tr}(D(B^T B)^{-1}) = \text{tr}(D G^{-1})$, thus proving the first equation for $\gamma_1(h, u)$ in (23). Similarly, $\text{tr}(D^2) = \text{tr}((C^T (B^{-1})^T D B^{-1} C)^2) = \text{tr}((D G^{-1})^2)$ for $\gamma_2(h, u)$. For $\gamma_3(h, u)$, applying the argument of $\gamma_1(h, u)$ twice to $(i, j)$ and $(k, l)$ in $\tilde{h}_{ijkl} \Delta u_i \Delta u_j \Delta u_k \Delta u_l = d_{ijkl} x_i x_j x_k x_l$, we get the last equation in (23).

For deriving the asymptotic expansions of $\gamma_i$'s in (24), we first consider $g_{ij} = b_i b_j = \delta_i \delta_j + (\delta_i / \partial u_i) (\partial h / \partial u_j) = \delta_{ij} + (2 h_{ik} u_k + O(n^{-1}))(2 h_{ij} u_l + O(n^{-1})) = \delta_{ij} + 4 h_{ik} h_{jl} u_k u_l + O(n^{-3/2})$. Since $(\theta_{ij} + \lambda)^{1/2} = \theta_{ij} - A^2 + O(\theta^4)$, the elements of $G^{-1}$ are $g^{ij} = \delta_{ij} - 4 h_{ik} h_{jl} u_k u_l + O(n^{-3/2})$. Noting the expression of $\tilde{h}_{ij}$ shown in Lemma 1, we have $\gamma_1(h, u) = \tilde{h}_{ij} g^{ij} \tilde{h}_{kl} g^{kl} = \tilde{h}_{ij} (\delta_{jk} + O(n^{-1})) \tilde{h}_{kl} (\delta_{ij} + O(n^{-1})) = \tilde{h}_{ijkl} (\delta_{ij} + O(n^{-1})) = \tilde{h}_{ijkl} (\delta_{ij} + O(n^{-3/2}))) = \tilde{h}_{ij} h_{ij} + 6 h_{ij} h_{ijk} u_k$. Similarly, $\gamma_3(h, u) = h_{ij} h_{ijk} h_{kl} + \gamma_3(h, u) \tilde{h}_{ijkl} \sim h_{ijkl}$. We leave terms such as $h_{lmn} h_{mjk} = O(n^{-3/2})$ in $a_{ijk}$ unsymmetrical with respect to permutation of indices for brevity. Next, we verify that

$$u_i = \theta_i - \lambda_0 h_i - 2 \lambda_0 h_{ij} j \theta_{ij} + 4 \lambda_0^2 h_{ij} h_{jk} \theta_{jk} - 3 \lambda_0 h_{ijk} \theta_{jk} + O(n^{-3/2})$$

is the solution of (40) up to $O(n^{-1})$ terms. Noting $\lambda(u) \|f\|^{-1} = \lambda_0 + O(n^{-1})$ and $\partial h / \partial u_i = h_i + 2 h_{ij} u_j + \lambda_0 h_{ij} h_{jk} \theta_{jk} + O(n^{-3/2})$, (40) is expressed as $\theta_i = u_i - \lambda_0 (h_i + 2 h_{ij} u_j + \lambda_0 h_{ij} h_{jk} \theta_{jk} + O(n^{-3/2}))) \{ \theta_j + O(n^{-1/2}) \} = u_i + \lambda_0 h_i + 2 \lambda_0 h_{ij} \theta_{ij} - 4 \lambda_0^2 h_{ij} h_{jm} \theta_{jk} + 3 \lambda_0 h_{ijk} \theta_{jk} + O(n^{-3/2}) = \theta_i + O(n^{-1/2})$, confirming the solution.

We then substitute (42) into $a_{ij} u_i + a_{ij} u_j + a_{jk} u_j u_k + a_{ikl} u_i u_j u_k$. They are $a_{ijk} \simeq (a_i - 2 \lambda_0 a_{ij} h_{jm} \theta_i) \theta_j + (a_j - 2 \lambda_0 a_{ij} h_{jm} \theta_i) \theta_k + 8 \lambda_0^2 a_{ij} h_{jm} \theta_i \theta_j \theta_k + (a_k - 4 \lambda_0 a_{ij} h_{jm} \theta_i) \theta_j \theta_k$, $a_{ijk} u_i u_j u_k \simeq a_{ijk} \theta_i \theta_j \theta_k \theta_i$, and $a_{ijkl} u_i u_j u_k u_l \simeq a_{ijkl} \theta_i \theta_j \theta_k \theta_l$. Rearranging the terms of $a(u)$, we get the expression of $s(\theta)$ with respect to $s_i$ as $s_i = \tilde{h}_{ij} - \lambda_0 - (h_i - \lambda_1 - 2 \lambda_0 h_{ij} (h_{jm} - \lambda_0 \theta_{ij})) \theta_j + (h_{ij} - \lambda_1 - 2 \lambda_0 h_{ij} h_{jm} + 4 \lambda_0^2 h_{ij} h_{jm} \theta_j \theta_j) \theta_j + (h_{ij} - 6 \lambda_0 h_{ij} h_{jm} \theta_j) \theta_k + h_{ijk} \theta_j \theta_k \theta_k$. Therefore, we obtain the coefficients $s_0$, $s_i$, $s_{ij}$ and $s_{ijk}$ as those given in the lemma. We also get $s_{ijk} = h_{ijk} - 6 \lambda_0 h_{ij} h_{jm} h_{mk}$, which becomes that given in the lemma by symmetrization with respect to permutation of indices.
Proof of Lemma 4. For \((\theta, -s(\theta))\) in (25), we will solve \(\text{BP}_{s}\langle \mathcal{R}(h)\rangle(\theta, -s(\theta)) = 1 - \alpha\) with respect to \(\lambda(u)\). We apply Theorem 2 to \(y = (\theta, -s(\theta))\). Let \(\tilde{\gamma}_i = \gamma_i(h, u), i = 1, \ldots, 4\) be the geometric quantities at \((u, -h(u)) = \hat{\mu}(H)(\theta, -s(\theta))\). It follows from (17) by replacing \(\lambda_0 \to \lambda(u), \gamma_i \to \tilde{\gamma}_i, h_i = h_i = 0\) that

\[
z_\alpha \simeq \sigma^{-1}\lambda(u) + \sigma\left(\tilde{\gamma}_1 - \lambda(u)\tilde{\gamma}_2 + \frac{4}{3}\lambda(u)^2\tilde{\gamma}_3\right) + \sigma^3\left(3\tilde{\gamma}_4 - \tilde{\gamma}_2 - \frac{4}{3}\tilde{\gamma}_3\right).
\]

Solving this equation with respect to \(\lambda(u)\), we obtain

\[
\lambda(u) \simeq \sigma z_\alpha - \sigma^2\tilde{\gamma}_1 + \sigma^2 z_\alpha\tilde{\gamma}_2 + \sigma^4\left(\frac{1}{3}(1 - z_\alpha^2)\tilde{\gamma}_3 - 3\tilde{\gamma}_4\right),
\]

which is easily verified by substituting (43) into the equation as \(z_\alpha \simeq \sigma^{-1}\lambda(u) + \sigma(\tilde{\gamma}_1 - (z_\alpha - \sigma^2\tilde{\gamma}_1 + O(n^{-1/2}))\tilde{\gamma}_2 + \frac{4}{3}(\sigma z_\alpha + O(n^{-1/2}))\tilde{\gamma}_3) + \sigma^3(3\tilde{\gamma}_4 - \tilde{\gamma}_2 - \frac{4}{3}\tilde{\gamma}_3) \simeq \sigma^{-1}\lambda(u) + \sigma^2\tilde{\gamma}_1 + \sigma^2(z_\alpha\tilde{\gamma}_2) + \sigma^4\left(\frac{4}{3}(z_\alpha^2 - 1)\tilde{\gamma}_3 + 3\tilde{\gamma}_4\right) \simeq z_\alpha\). Substituting (24) for \(\tilde{\gamma}_i = \gamma_i(h, u)\) in (43), we have \(\lambda_0 = \lambda(h, u), \lambda_i = -3\sigma^2h_{mm1} + 6\sigma^3z_\alpha h_{ml}h_{mli}\) and \(\lambda_{ij} = \sigma(\frac{-6h_{mmij} + 2h_{mmhij} + 4h_{mlhmi}h_{ij}}{3})\). For proving \((26)\), we eliminate a from \(z_\alpha\) by \(z_\alpha = \sigma^{-1}\lambda_0(1 + O(n^{-1/2}))\), and we get \(\lambda_i = \sigma^2(-3h_{mm} + 6h_{ml}h_{mli})\). By applying Theorem 3 to this \(\lambda(u)\), we obtain (27) and (28); actually we only have to check \(x_i, y_{ij}\), and \(\gamma_1(s, 0)\) as follows. \(x_i = h_i - \sigma^2(-3h_{mm} + 6h_{ml}h_{mli}) - 2\sigma h_{ml}(h_{mm} - \sigma^2(-3h_{ml} + O(n^{-1/2}))), \gamma_{ij} = \gamma_{ij} - \sigma^2(-6h_{mm} + 2h_{ml}h_{mj} + 4h_{mlhmi}h_{ij} + 2\sigma h_{ml}h_{mj} + 4\sigma^2h_{mlhml}h_{ij}), \) and \(\gamma_1(s, 0) = \gamma_1 - \lambda_i - \lambda_0, 2\lambda_0\gamma_2 + 4\lambda_0^2\gamma_3\) with \(\lambda_i = \gamma^2(-6\gamma_4 + 2\gamma_1\gamma_2 + 4\gamma_3) = \gamma^2-\beta_3\).

Proof of Lemma 5. Let \(s = \text{L}_{s2}(h, \lambda_0)\) and \(r = \text{L}_{r2}(s, \xi_0)\). Applying Lemma 4 to \(r\), we have the coefficients of \(r\) in terms of \(s\) and \(\xi_0\) such as \(r_0 = s_0 - \xi_0\) from (27). Then substitute the coefficients of \(s\) in terms of \(h\) and \(\lambda_0\), such as \(s_0 = h_0 - \lambda_0\), into those of \(r\) to get, say, \(r_0 = (h_0 - \lambda_0) - \xi_0 = h_0 - (\lambda_0 + \xi_0)\). After rearranging terms, we get the other coefficients as \(r_{ij} = h_{ij} - 2(\lambda_0 + \xi_0)h_{mlh_{mj}} + 4(\lambda_0 + \xi_0)h_{ml}h_{mli}h_{ij} + (\sigma^2 + \tau^2)(6h_{mm} - 2h_{mlh_{mj}} + h_{mlh_{mi}}h_{ij})\), \(r_{ijk} = h_{ijk} - 2(\lambda_0 + \xi_0)(h_{mlh_{mk}h_{mj} + h_{ml}h_{mj}h_{mk} + h_{mlh_{mk}h_{ij}}})\), \(r_{ijkl} = h_{ijkl}\). The additivity in terms of \(\sigma^2 + \tau^2\) and \(\lambda_0 + \xi_0\) holds for these four coefficients, thus proving (30). For \(r_1 = h_1 - 2(\lambda_0 + \xi_0)h_{mlh_{mj}} + (\sigma^2 + \tau^2)(3h_{mm} - 6(\lambda_0 + \xi_0)h_{mmh_{ml}h_{ij}} - 6(\lambda_0 + \xi_0)h_{mlh_{mi}h_{mj}} + (\sigma^2 - \tau^2)\lambda_0)h_{ml}\text{ml},\) the additivity holds except for the last term. Thus \(\gamma^2 = \gamma^2\) in (30) is replaced by \(\gamma^2\) when \(\sigma^2\xi_0 - \tau^2\lambda_0 = 0\). In particular, \(\text{L}_{s2}(s_0, \lambda_0) \simeq \text{L}_{s2}(0, 0) \simeq h_0\).

Proof of Theorem 3. We only have to show that \(\gamma_i \to \gamma_i(s, 0), \lambda_0 \to -\lambda_0\) with \(s = \text{L}_{s2}(h, \lambda_0)\) leads to \(\beta_0 \to -\beta_0, \beta_1 \to \beta_1 - \beta_3, \beta_2 \to \beta_2\) as mentioned just before the theorem. Here we show a generalized result for \(s = \text{L}_{s2}(h, \lambda_0)\) to be used later again. The geometric quantities are given in (28) of Lemma 4. We replace \(\gamma_i \to \gamma_i(s, 0)\) and \(\lambda_0 \to -\lambda_0\) in \(\beta_0, \beta_1, \beta_2\) of (11). They become \(\beta_0 \to -\lambda_0 = -\beta_0, \beta_1 \to \gamma_1 + 2\lambda_0\gamma_2 + 4\lambda_0^2\gamma_3 + \sigma^2\beta_3 - (\lambda_0)\gamma_2 - 4\lambda_0^2\gamma_3 + \frac{4}{3}(\lambda_0)\gamma_3 + \sigma^2\beta_3 = \beta_1 + \sigma^2\beta_3, \beta_2 \to 3\lambda_0 + (\gamma_1 + O(n^{-1/2}))\gamma_2 + O(n^{-1/2})) - \frac{4}{3}\gamma_3 \simeq \beta_2\).

Proof of Theorem 4. We first consider the case of \(\tilde{\mu} = (0, -h_0)\) with \(\theta = 0\). For applying Theorem 2 to \(\text{BP}_{s2}(\mathcal{R}(s))(0, -h_0)\) with \(s = \text{L}_{s2}(h, \lambda_0)\), we would like to replace \(h \to s\) and \(\lambda_0 \to -\lambda_0\) in \(\text{BP}_{s2}(\mathcal{R}(h))(0, \lambda_0 - h_0)\). We replace \(\sigma^2 \to \tau^2, \gamma_i \to \gamma_i(s, 0), \lambda_0 \to -\lambda_0\) in (17). This results in \(\beta_0 \to -\beta_0, \beta_1 \to \beta_1 + \sigma^2\beta_3, \beta_2 \to \beta_2\) as shown in the proof of Theorem 3, and thus \(\text{DBP}_{s2, s2}(H|y) \simeq 1 - \Phi((-\beta_0)\tau^{-1} + (\beta_1 + \sigma^2\beta_3)\tau + \beta_2\tau^3)\), giving the right hand side of (32).

Next, we compute \(\text{DBP}_{s2, s2}(H|y)\) with \(\tilde{\mu} = (\theta, -h(\theta))\) for \(\theta = O(1)\). We only have to replace \(\beta_0, \ldots, \beta_3\) in (32) by those evaluated at \(\tilde{\mu}_1, \ldots, \beta_3\). Replacing \(\lambda_0 \to \lambda_{s2}(\theta), \gamma_i \to \gamma_i(h, \theta)\) in (11), we have \(\tilde{\beta}_0 = \lambda_{s2}(\theta) = \gamma_0 - \sigma^2\gamma_0, \tilde{\beta}_1 \simeq \gamma_1(h, \theta) - \lambda_{s2}(\theta)\gamma_2(h, \theta) + \ldots \)
\[ 4\lambda_{\sigma}(\theta)^2 \gamma_3(\theta, \gamma) = \beta_1 + \kappa(\theta), \quad \beta_2 \simeq \beta_2, \quad \beta_3 \simeq \beta_3. \] Therefore, \( \text{DBP}_{\sigma, \sigma}^2(H)(y) \simeq \Phi((\beta_0 - \sigma^2 \kappa(\theta)) \tau^{-1} - (\beta_1 + \kappa(\theta)) \tau - \beta_2 \tau^2 - \beta_3 \tau^3)) \), giving (31).

**Proof of Theorem 5.** Let \( \lambda_0 \in \mathbb{R} \) be the solution of the equation \( \text{NBP}_{\sigma}(H)(0, \lambda_0 - h_0) = \alpha \). From (18), the equation is expressed as \( \beta_0 + \beta_1 \sigma^2 + \beta_2 \sigma^4 \simeq -z_\alpha \) with (11). By solving it with respect to \( \lambda_0 \), we get \( \lambda_0 = -z_\alpha - \sigma^2 (\gamma_1 + z_\alpha \gamma_2 + \frac{3}{4} z_\alpha^2 \gamma_3) - \sigma^4 (3 \gamma_4 - \frac{3}{4} \gamma_5) \). This is easily verified by substituting it into the left hand side of the equation as \( \lambda_0 + \sigma^2 (\gamma_1 - (-z_\alpha - \sigma^2 \gamma_1) \gamma_2 + \frac{3}{8} (z_\alpha - \sigma^2 \gamma_2) \gamma_3 + \sigma^4 \beta_2 \simeq -z_\alpha \). For \( \bar{\mu} = (0, -h_0) \), the right hand side of (32) gives \( \text{DBP}_{1, \sigma}^2(H)(0, \lambda_0 - h_0) \simeq \Phi(-\beta_0 + \beta_1 + \beta_2 + \sigma^2 \beta_3) \simeq \Phi(-\lambda_0 + \gamma_1 - (z_\alpha - \sigma^2 \gamma_1) \gamma_2 + \frac{3}{8} (z_\alpha - \sigma^2 \gamma_2) \gamma_3 + \sigma^4 \beta_3) \). This becomes (33) by collecting terms with respect to \( \sigma^2 \) after substituting the expression of \( \lambda_0 \).

**Proof of Theorem 6.** Let \( \lambda_0 \in \mathbb{R} \) be the solution of the equation \( \text{DBP}_{1, \sigma}(H)(0, \lambda_0 - h_0) = \alpha \). From (32), the equation is expressed as \( \beta_0 - \beta_1 - \beta_2 - \sigma^2 \beta_3 \simeq -z_\alpha \) with (11). By solving it with respect to \( \lambda_0 \), we get \( \lambda_0 = -z_\alpha + \gamma_1 + z_\alpha \gamma_2 - 2 \gamma_1 \gamma_2 + 3 \gamma_4 + \frac{3}{4} \gamma_3 (z_\alpha^2 - 1) + \sigma^2 \beta_3 \). We define \( \lambda \in \mathcal{S} \) by substituting \( \gamma_i(h, u) \) for \( \gamma_i \) in the expression of \( \lambda_0 \). Then \( \lambda(u) \simeq -z_\alpha + \gamma_1 (h, u) + z_\alpha \gamma_2 (h, u) - 2 \gamma_1 \gamma_2 + 3 \gamma_4 + \frac{3}{4} \gamma_3 (z_\alpha^2 - 1) + \sigma^2 \beta_3 \simeq \lambda_0 + 3(h_{mmn} + 6z_\alpha h_{nmi} u_i + (6h_{nmm} - 2 h_{mlj} h_{mni} - 4 h_{mli} h_{mij}) u_j) u_j \). Noting \( z_\alpha = -\lambda_0 + O(n^{-1/2}) \), we find \( \lambda(u) \simeq \lambda_0 + \kappa(u) \), where \( \kappa(u) \) is defined in (29). Using this \( \lambda(u) \), the contour surface \( \text{DBP}_{1, \sigma}^2(H)(y) = \alpha \) is expressed as \( y \in \mathcal{B}(s) \) for \( s = \mathcal{M}(h, \lambda) \simeq \mathcal{L}_{-1}(h, \lambda_0) \). For \( \bar{\mu} = (0, -h_0) \), the right hand side of (32) gives \( \text{DBP}_{1, \sigma}^2(H)(0, \lambda_0 - h_0) \simeq \Phi(-\beta_0 + \beta_1 + \beta_2 - \beta_3) \simeq \Phi(-\lambda_0 + \gamma_1 - (z_\alpha + \gamma_1) \gamma_2 + \frac{3}{8} (z_\alpha - \sigma^2 \gamma_2) \gamma_3 + \sigma^4 \beta_3) \simeq \Phi(z_\alpha - (1 + \sigma^2) \beta_3) \), showing (34).

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