

BEST INVARIANT ESTIMATION OF A DISTRIBUTION FUNCTION UNDER THE KOLMOGOROV–SMIRNOV LOSS FUNCTION¹

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Given a random sample of size n from an unknown continuous distribution function F , we consider the problem of estimating F nonparametrically from a decision theoretic approach. In our treatment, we assume the Kolmogorov–Smirnov loss function and the group of all one-to-one monotone transformations of real numbers onto themselves which leave the sample values invariant. Under this setup, we obtain a best invariant estimator of F which is shown to be unique. This estimator is a step function with unequal amounts of jumps at the observations and is an improper distribution function. It is remarked that this estimator may be used in constructing the best invariant confidence bands for F , and also in carrying out a goodness-of-fit test.

1. Introduction. Given a random sample of size n from an unknown continuous cumulative distribution function (cdf) F , we consider the problem of estimating F . To evaluate the discrepancy between F and its estimator, several loss functions are available in the literature. Aggarwal (1955) considered the Cramer–von Mises type of loss functions

$$(1.1) \quad L(F, \hat{F}) = \int |F(x) - \hat{F}(x)|^r \psi(F(x)) dF(x),$$

where ψ is a specific function of $F(x)$ and r is a positive integer, and obtained best invariant estimators under the group of all one-to-one monotone transformations. In particular, he showed that the sample cdf is the best invariant estimator under the preceding loss function with $\psi(x) = [x(1-x)]^{-1}$. Using a similar approach, Phadia (1974) derived a set of best invariant one and two sided confidence bands for F . Only recently, Brown (1984) gave a formulation and obtained some partial results when F is not assumed to be continuous.

Phadia (1973) assumed a noninvariant loss function of the type

$$\int (F - \hat{F})^2 \psi(F) dW,$$

where W is a known nonnull measure on \mathbb{R}^1 . Without assuming the continuity of

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F , he obtained minimax estimators. In particular, he showed that the sample cdf is minimax when $\psi(x) = [x(1 - x)]^{-1}$. (For the invariant loss function (1.1), it is an open question whether the best invariant estimator is minimax [see Ferguson (1967)]. Recently, Yu (1986a, b) announced some partial results in this direction.)

Another type of loss function which is also invariant under the group of transformations is the Kolmogorov–Smirnov loss function given by

$$(1.2) \quad L(F, \hat{F}) = \sup_x |F(x) - \hat{F}(x)|.$$

This loss function is difficult to handle analytically and until recently no results were available on the estimation of F using this loss function. Recently, Brown (1984) reported the best invariant estimator under this loss function, but only for the case $n = 1$.

Our objective in this paper is to obtain the best invariant estimator under this loss function for any finite sample size.

2. The main result. We consider the following decision theoretic structure:

$$\mathcal{F} = \left\{ \begin{array}{l} F: F \text{ is a continuous cumulative distribution function defined} \\ \text{on the real line } \mathbb{R}^1 \end{array} \right\},$$

$$\mathcal{A} = \left\{ \begin{array}{l} \Phi: \Phi \text{ is a right continuous cumulative distribution function on} \\ \mathbb{R}^1 \text{ such that } 0 \leq \Phi(-\infty) < \Phi(+\infty) \leq 1 \end{array} \right\}.$$

The loss function is given by $L(F, \Phi) = \sup_x |F(x) - \Phi(x)|$ for $F \in \mathcal{F}$ and $\Phi \in \mathcal{A}$.

\mathcal{X} is the sample space for samples of size n , $\mathcal{X} \subset \mathbb{R}^n$. Let δ be a decision rule, $\delta: \mathcal{X} \rightarrow \mathcal{A}$. Define the risk function of the decision rule δ (or \hat{F}) by

$$R(F, \delta) = E(L(F, \delta(\cdot))) = E(L(F, \hat{F})).$$

Let $x_1 \leq x_2 \leq \dots \leq x_n$ be an ordered sample from $F \in \mathcal{F}$. Since the vector of order statistics is sufficient for F , it is enough to consider only the estimators which are functions of the order statistics. Also, it is well known [see, for example, Aggarwal (1955) or Ferguson (1967) for a formal proof] that the only procedures which are invariant under the group of transformations

$$\mathcal{G} = \left\{ \begin{array}{l} g_\varphi: g_\varphi(x_1, \dots, x_n) = (\varphi(x_1), \dots, \varphi(x_n)) \text{ and } \varphi \text{ is a} \\ \text{continuous strictly increasing function from } \mathbb{R}^1 \text{ onto } \mathbb{R}^1 \end{array} \right\}$$

are of the form

$$(2.1) \quad \hat{F}(x) = \sum_{j=1}^{n+1} u_j 1_{[x_{j-1}, x_j)}(x),$$

where $1_A(\cdot)$ is the indicator function of the set A , the u_j 's are constants, $x_0 = -\infty$ and $x_{n+1} = +\infty$. Clearly, $\hat{F} \in \mathcal{A}$. Thus, to find the best invariant estimator, we have to determine the u_j 's suitably.

Our main result is

THEOREM 1. *Let $x_1 \leq x_2 \leq \dots \leq x_n$ be an ordered sample from $F \in \mathcal{F}$. Then, under the loss function L , the action space \mathcal{A} and the group of*

TABLE 1
Optimal values of \bar{u}_i

| $n \backslash i$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 1 | 0.3750 | | | | | | | | | |
| 2 | 0.2929 | | | | | | | | | |
| 3 | 0.2441 | 0.4013 | | | | | | | | |
| 4 | 0.2072 | 0.3366 | | | | | | | | |
| 5 | 0.1903 | 0.2956 | 0.4295 | | | | | | | |
| 6 | 0.1724 | 0.2608 | 0.3759 | | | | | | | |
| 7 | 0.1567 | 0.2338 | 0.3351 | 0.4448 | | | | | | |
| 8 | 0.1483 | 0.2166 | 0.3024 | 0.3989 | | | | | | |
| 9 | 0.1361 | 0.1966 | 0.2766 | 0.3644 | 0.4553 | | | | | |
| 10 | 0.1263 | 0.1817 | 0.2567 | 0.3350 | 0.4175 | | | | | |
| 11 | 0.1212 | 0.1708 | 0.2362 | 0.3106 | 0.3858 | 0.4613 | | | | |
| 12 | 0.1148 | 0.1611 | 0.2222 | 0.2888 | 0.3568 | 0.4295 | | | | |
| 13 | 0.1096 | 0.1517 | 0.2075 | 0.2697 | 0.3327 | 0.3994 | 0.4662 | | | |
| 14 | 0.1050 | 0.1440 | 0.1954 | 0.2537 | 0.3131 | 0.3763 | 0.4373 | | | |
| 15 | 0.1000 | 0.1358 | 0.1854 | 0.2391 | 0.2952 | 0.3538 | 0.4117 | 0.4705 | | |
| 16 | 0.0960 | 0.1317 | 0.1756 | 0.2255 | 0.2789 | 0.3336 | 0.3885 | 0.4442 | | |
| 17 | 0.0914 | 0.1246 | 0.1666 | 0.2670 | 0.3183 | 0.3693 | 0.4206 | 0.4732 | | |
| 18 | 0.0904 | 0.1198 | 0.1604 | 0.2065 | 0.2537 | 0.3027 | 0.3512 | 0.4008 | 0.4501 | |
| 19 | 0.0869 | 0.1151 | 0.1545 | 0.1971 | 0.2423 | 0.2880 | 0.3347 | 0.3814 | 0.4290 | 0.4762 |
| 20 | 0.0821 | 0.1109 | 0.1470 | 0.1882 | 0.2313 | 0.2756 | 0.3195 | 0.3639 | 0.4088 | 0.4544 |
| 25 ^a | 0.0718 | 0.0942 | 0.1236 | 0.1557 | 0.1897 | 0.2247 | 0.2609 | 0.2972 | 0.3338 | 0.3707 |
| | 0.4076 | 0.4446 | 0.4815 | | | | | | | |

^aThe second row for $n = 25$ contains values for u_i , $i = 11, 12$ and 13 .

transformations \mathcal{G} , the best invariant estimator of F is unique and given by (2.1), where the constants u_j are

$$\begin{aligned}
 &\text{for } n = 1, && u_1 = 3/8 \text{ and } u_2 = 1 - u_1 = 5/8, \\
 &\text{for } n = 2, && u_1 = 1 - 1/\sqrt{2}, \quad u_2 = 1/2, \quad u_3 = 1 - u_1 = 1/\sqrt{2}, \\
 &\text{for } n \geq 3, \\
 (2.2) \quad &&& u_j = 1 - u_{n+2-j}, \quad j = 1, 2, \dots, [(n + 1)/2].
 \end{aligned}$$

The values of u_j for $j \leq n/2$ are given in Table 1 and for $j > n/2$ can be calculated from (2.2).

REMARKS. The estimator is of course a step function with positive masses at the observations only. Like most of the best invariant estimators and the minimax estimator referenced earlier, it is also an improper distribution function. However, unlike them, the amounts of jumps at the observations are not constant but increase toward the midpoint. It is also symmetric about the middle.

For the sample sizes $n = 1$ and 2 , we have exact results. For $n \geq 3$, the task becomes very difficult, and therefore we have used an algorithm to compute the u_j 's on a computer. It would be interesting to discover a formula to calculate the

sizes of jumps as in the case of the abovementioned estimators. However, it is doubtful whether any such formula can be discovered in a closed form.

To prove the theorem, we need several preliminary results.

Since F is assumed to be continuous, by using the probability integral transformation we may rewrite the risk of $\hat{F} \in \mathcal{A}$, given in (2.1) as

$$\begin{aligned}
 R(F, \delta) &= E[L(F, \delta(\cdot))] = E\left[\sup_x \left|F(x) - \sum_{j=1}^{n+1} u_j 1_{[x_{j-1}, x_j)}(x)\right|\right] \\
 (2.3) \quad &= E\left[\sup_t \left|t - \sum_{j=1}^{n+1} u_j 1_{[y_{j-1}, y_j)}(t)\right|\right] \\
 &= n! \int_{\Omega} l(\bar{u}, \bar{y}) \, d\bar{y} \equiv n! \varphi(\bar{u}),
 \end{aligned}$$

where $\bar{u} = (u_1, \dots, u_{n+1})$, $\bar{y} = (y_1, \dots, y_n)$,

$$(2.4) \quad l(\bar{u}, \bar{y}) = \sup_t \left|t - \sum_{j=1}^{n+1} u_j 1_{[y_{j-1}, y_j)}(t)\right|$$

and

$$(2.5) \quad \Omega = \{\bar{y} \in \mathbb{R}^n \mid 0 = y_0 \leq y_1 \leq \dots \leq y_n \leq y_{n+1} = 1\}.$$

The expectation in the third equation is taken with respect to the uniform distribution on $I^n \equiv [0, 1]^n$.

Next we note that the supremum in (2.4) is achieved at $t = y_i$ for some $i = 0, 1, 2, \dots, n + 1$. Define the distances between t and the estimator by

$$(2.6) \quad l_i(\bar{u}, \bar{y}) = \begin{cases} u_i - y_{i-1}, & \text{for } i = 1, 2, \dots, n + 1, \\ y_{i-n-1} - u_{i-n-1}, & \text{for } i = n + 2, \dots, 2n + 2. \end{cases}$$

We thus get $l(\bar{u}, \bar{y}) = \max_{1 \leq i \leq 2n+2} \{|l_i(\bar{u}, \bar{y})|\}$.

For $i = 2, \dots, 2n + 1$ and for $i = 1, 2n + 2$ when $u_1 \neq 1 - u_{n+1}$, define Ω_i by

$$(2.7) \quad \Omega_i(\bar{u}) = \{\bar{y} \in \Omega \mid l_i(\bar{u}, \bar{y}) > |l_j(\bar{u}, \bar{y})|, j \neq i, j = 1, \dots, 2n + 2\},$$

on which $l(\bar{u}, \bar{y}) = l_i(\bar{u}, \bar{y})$.

When $i = 1, 2n + 2$ and $u_1 = 1 - u_{n+1}$, we define

$$\Omega_1(\bar{u}) \cup \Omega_{2n+2}(\bar{u}) = \{\bar{y} \in \Omega \mid l_1(\bar{u}, \bar{y}) = l_{2n+2}(\bar{u}, \bar{y})\}.$$

Note that the Ω_i 's are disjoint sets and $\cup_{i=1}^{2n+2} \Omega_i = \Omega$.

LEMMA 1. *The risk function $\varphi(\bar{u})$ is strictly convex for*

$$\bar{u} \in \bar{\Lambda} \equiv \{\bar{u} \in I^{n+1} \mid 0 \leq u_1 \leq u_2 \leq \dots \leq u_{n+1} \leq 1\}.$$

PROOF. Let $\bar{u}, \bar{w} \in \bar{\Lambda}$, $\bar{u} \neq \bar{w}$ and $\lambda \in (0, 1)$. Since by (2.6) all $l_i(\bar{u}, \bar{y})$ are affine functions in \bar{u} , for any fixed $\bar{y} \in \Omega$ we have

$$\begin{aligned}
 l(\lambda \bar{u} + (1 - \lambda)\bar{w}, \bar{y}) &= \max_i \{|l_i(\lambda \bar{u} + (1 - \lambda)\bar{w}, \bar{y})|\} \\
 &= \max_i \{|\lambda l_i(\bar{u}, \bar{y}) + (1 - \lambda)l_i(\bar{w}, \bar{y})|\} \\
 (2.8) \qquad &\leq \lambda \max_i |l_i(\bar{u}, \bar{y})| + (1 - \lambda) \max_j |l_j(\bar{w}, \bar{y})| \\
 &= \lambda l(\bar{u}, \bar{y}) + (1 - \lambda)l(\bar{w}, \bar{y}),
 \end{aligned}$$

and equality occurs if and only if $y \in \Omega_i(\bar{u}) \cap \Omega_i(\bar{w})$ for some given i .

Since $\bar{u} \neq \bar{w}$, it can be shown that there is an index i for which $\Omega_i(\bar{u}) \neq \Omega_i(\bar{w})$ and strict inequality in (2.8) will hold for \bar{y} on a set of positive measure in Ω . Thus,

$$\begin{aligned}
 \varphi(\lambda \bar{u} + (1 - \lambda)\bar{w}) &= \int_{\Omega} l(\lambda \bar{u} + (1 - \lambda)\bar{w}, \bar{y}) \, d\bar{y} \\
 &< \lambda \int_{\Omega} l(\bar{u}, \bar{y}) \, d\bar{y} + (1 - \lambda) \int_{\Omega} l(\bar{w}, \bar{y}) \, d\bar{y} \\
 &= \lambda \varphi(\bar{u}) + (1 - \lambda)\varphi(\bar{w}),
 \end{aligned}$$

proving the lemma. \square

Since the problem is invariant under reflection which maps $x_i \rightarrow 1 - x_{n-i+1}$, the minimum of the convex function $\varphi(\bar{u})$ will occur at a point \bar{u} invariant under this reflection. Taking into account the definition of l , this means that the minimum of φ occurs at a point satisfying $\bar{u}_i = 1 - \bar{u}_{n-i+2}$. Thus introduce new variables

$$\begin{aligned}
 \bar{z} \in U_m &= \{(z_1, z_2, \dots, z_m) \mid 0 \leq z_1 \leq z_2 \leq \dots \leq z_m \leq 1\} \\
 &\qquad \qquad \qquad \text{with } m = \left\lfloor \frac{n+1}{2} \right\rfloor.
 \end{aligned}$$

Define a mapping $\bar{u}(\bar{z})$ from U_m to Λ as follows: If n is even, $u_i = z_i$, $i = 1, 2, \dots, m$, $u_i = 1 - u_{n-i+2}$, $i = m + 2, \dots, n + 1$ and $u_{m+1} = 1/2$; if n is odd, $u_i = z_i$, $i = 1, 2, \dots, m$ and $u_i = 1 - u_{n-i+2}$, $i = m + 1, \dots, n + 1$. Let $\varphi(\bar{z}) = \varphi(\bar{u}(\bar{z}))$.

Since the mapping $\bar{u}(\bar{z})$ is a linear mapping, it follows from Lemma 1 that $\varphi(\bar{z})$ is strictly convex on U_m . Thus [see, for example, Roberts and Verberg (1973), Theorems A and B, page 123] any local minimum of $\varphi(\bar{u})$ is also a global one. From the abovementioned symmetry, this minimum occurs at some point $\bar{u}(\bar{z})$. Moreover, if $\text{grad } \varphi(\bar{z}) = 0$ for some \bar{z} , then $\bar{u}(\bar{z})$ is the minimal point of $\varphi(\bar{u})$.

The next theorem gives expressions for the $\text{grad } \varphi(\bar{u})$ and $\text{grad } \varphi(\bar{z})$.

THEOREM 2. *Let $\varphi(\bar{u})$ and $\Omega_i(\bar{u})$ be as defined in (2.3) and (2.7), respectively. Then*

$$(2.9) \quad \frac{\partial \varphi(\bar{u})}{\partial u_k} = [V(\Omega_k) - V(\Omega_{n+k+1})], \quad k = 2, 3, \dots, n,$$

where $V(\Omega_i)$ stands for the volume of the set Ω_i , $i = 2, \dots, 2n + 1$, and with $V(\Omega_1) = V(\Omega_{2n+2}) = \frac{1}{2}V(\Omega_1 \cup \Omega_{2n+2})$. In addition, if $\varphi(\bar{z})$ is as previously defined, then $\varphi(\bar{z})$ is differentiable at any $\bar{z} \in U_m^0$, interior of U_m and

$$(2.10) \quad \frac{\partial \varphi(\bar{z})}{\partial z_k} = 2[V(\Omega_k) - V(\Omega_{n+k+1})], \quad k = 1, 2, \dots, m.$$

Moreover, this formula is also valid on $\partial U_m = U_m - U_m^0$ when the derivative is interpreted as a one sided derivative.

PROOF. For $k = 2, 3, \dots, n$ denote by $\overline{\Delta u}_k$ a $(n + 1)$ -dimensional vector with Δu_k at the k th position and zero elsewhere. By using (2.7), we have

$$(2.11) \quad \begin{aligned} \varphi(\bar{u} + \overline{\Delta u}_k) - \varphi(\bar{u}) &= \int_{\Omega} [l(\bar{u} + \overline{\Delta u}_k, \bar{y}) - l(\bar{u}, \bar{y})] d\bar{y} \\ &= \sum_{i=1}^{2n+2} \int_{\Omega_i} \Delta_k l(\bar{u}, \bar{y}) d\bar{y} \\ &= \sum_{i=1}^{2n+2} \left[\int_{\Omega_i \cap \Omega'_i} \Delta_k l d\bar{y} + \int_{\Omega_i \setminus \Omega'_i} \Delta_k l d\bar{y} \right], \end{aligned}$$

where $\Delta_k l(\bar{u}, \bar{y}) = l(\bar{u} + \overline{\Delta u}_k, \bar{y}) - l(\bar{u}, \bar{y})$, $\Omega_i = \Omega_i(\bar{u})$ and $\Omega'_i = \Omega_i(\bar{u} + \overline{\Delta u}_k)$.

For $i \neq k$ or $n + k + 1$ and $\bar{y} \in \Omega_i \cap \Omega'_i$, $l(\bar{u} + \overline{\Delta u}_k, \bar{y}) = l_i(\bar{u} + \overline{\Delta u}_k, \bar{y}) = l_i(\bar{u}, \bar{y}) = l(\bar{u}, \bar{y})$ and, therefore, $\Delta_k l(\bar{u}, \bar{y}) = 0$. For $\bar{y} \in \Omega_k \cap \Omega'_k$, by (2.6)

$$(2.12) \quad \begin{aligned} \Delta_k l(\bar{u}, \bar{y}) &= l_k(\bar{u} + \overline{\Delta u}_k, \bar{y}) - l_k(\bar{u}, \bar{y}) \\ &= (u_k + \Delta u_k - y_{k-1}) - (u_k - y_{k-1}) = \Delta u_k. \end{aligned}$$

Similarly, for $\bar{y} \in \Omega_{n+k+1} \cap \Omega'_{n+k+1}$,

$$\Delta_k l(\bar{u}, \bar{y}) = -\Delta u_k.$$

Thus, (2.11) can be written in the form

$$(2.13) \quad \begin{aligned} \varphi(\bar{u} + \overline{\Delta u}_k) - \varphi(\bar{u}) &= \Delta u_k \left[\int_{\Omega_k \cap \Omega'_k} d\bar{y} - \int_{\Omega_{n+k+1} \cap \Omega'_{n+k+1}} d\bar{y} \right] \\ &+ \sum_{i=1}^{2n+2} \int_{\Omega_i \setminus \Omega'_i} \Delta_k l(\bar{u}, \bar{y}) d\bar{y} \\ &= \Delta u_k [V(\Omega_k \cap \Omega'_k) - V(\Omega_{n+k+1} \cap \Omega'_{n+k+1})] \\ &+ \sum_{i=1}^{2n+2} \int_{\Omega_i \setminus \Omega'_i} \Delta_k l(\bar{u}, \bar{y}) d\bar{y}. \end{aligned}$$

Obviously, by (2.6) and (2.7),

$$\lim_{\Delta u_k \rightarrow 0} [V(\Omega_k \cap \Omega'_k) - V(\Omega_{n+k+1} \cap \Omega'_{n+k+1})] = [V(\Omega_k) - V(\Omega_{n+k+1})].$$

It can be shown that

$$\sum_{i=1}^{2n+2} \int_{\Omega_i \setminus \Omega'_i} \Delta_k l(\bar{u}, \bar{y}) d\bar{y} = O((\Delta u_k)^2).$$

We omit the details. Finally, (2.13) implies (2.9) and, by using the chain rule, (2.9) yields (2.10). \square

PROOF OF THEOREM 1. From (2.3), it follows that in order to determine the best invariant estimator, we have to find a \bar{u} minimizing $\varphi(\bar{u})$ on $\bar{\Lambda}$. Strict convexity of $\varphi(\bar{u})$ (Lemma 1) and the symmetry imply that this unique minimum occurs at a vector \bar{u} of the form $\bar{u}(\bar{z})$, where \bar{z} is the unique minimum of $\varphi(\bar{z})$ on U_m . Using (2.10), it can be shown that this minimum does not occur on ∂U_m . Since $\varphi(\bar{z})$ is differentiable, this \bar{z} is the unique solution of the equation $\text{grad } \varphi(\bar{z}) = 0$ or equivalent to the solution of the system of equations

$$(2.14) \quad V(\Omega_k(\bar{u}(\bar{z}))) = V(\Omega_{n+k+1}(\bar{u}(\bar{z}))), \quad k = 1, 2, \dots, m.$$

For $n = 1$, this solution recapitulates the result of Brown (1984).

For $n = 2$, the sets $\Omega_i, i = 1, 2, \dots, 6$, are sketched in Figure 1. Equation (2.14) reduces to $V(\Omega_1) = V(\Omega_4)$, leading to the quadratic equation $2z_1^2 - 4z_1 + 1 = 0$, which yields the solution $z_1 = 1 - 1/\sqrt{2}$.

For $n = 3$, this calculation leads to a system of two equations in two variables each of order 3, which cannot be solved analytically. But since $\varphi(\bar{z})$ is convex and (2.10) gives the explicit formula for $\text{grad } \varphi(\bar{z})$, the unconstrained gradient search procedure can be applied to find the minimum of $\varphi(\bar{z})$. The calculations of optimal \bar{z} 's, for $n \leq 20$ and $n = 25$, were performed on the computer, using IMSL routine ZXCGR, based on a conjugate gradient algorithm described in

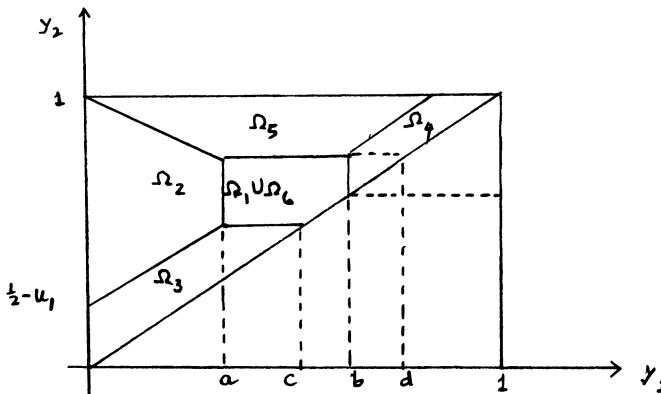


FIG. 1.

Powell (1977). The data in Table 1 are calculated under stopping criterion $|\text{grad } \varphi(\bar{z})| \leq 10^{-8}$. \square

REMARK. Using this best invariant estimator in place of the sample distribution function, one may construct the best invariant confidence bands, as in Phadia (1974), under the Kolmogorov–Smirnov loss function. However, the calculations are difficult. Partial results have been obtained by the authors. Furthermore, one may use this estimator in constructing a test statistic, similar to the Kolmogorov–Smirnov statistic, to carry out a goodness-of-fit test. This idea will be developed in a separate paper.

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