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# Computing the Kolmogorov-Smirnov Distribution when the Underlying Cdf is Purely Discrete, Mixed or Continuous 

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#### Abstract

The distribution of the Kolmogorov-Smirnov (K-S) test statistic has been widely studied under the assumption that the underlying theoretical cdf, $F(x)$, is continuous. However, there are many real-life applications in which fitting discrete or mixed distributions is required. Nevertheless, due to inherent difficulties, the distribution of the K-S statistic when $F(x)$ has jump discontinuities has been studied to a much lesser extent and no exact and efficient computational methods have been proposed in the literature.

In this paper, we provide a fast and accurate method to compute the (complementary) cdf of the K-S statistic when $F(x)$ is discontinuous, and thus obtain exact $p$ values of the K-S test. Our approach is to express the complementary cdf through the rectangle probability for uniform order statistics, and to compute it using Fast Fourier Transform (FFT). Secondly, we provide a C++ and an R implementation of the proposed method, which fills in the existing gap in statistical software. We give also a useful extension of the Schmid's asymptotic formula for the distribution of the K-S statistic, relaxing his requirement for $F(x)$ to be increasing between jumps and thus allowing for any general mixed or purely discrete $F(x)$. The numerical performance of the proposed FFT-based method, implemented both in C++ and in the R package KSgeneral, available from https: //CRAN.R-project.org/package=KSgeneral, is illustrated when $F(x)$ is mixed, purely discrete, and continuous. The performance of the general asymptotic formula is also studied.


Keywords: Kolmogorov-Smirnov test statistic, discontinuous (discrete or mixed) distribution, Fast Fourier Transform, double boundary non-crossing, rectangle probability for uniform order statistics.

## 1. Introduction

The two-sided Kolmogorov-Smirnov (K-S) statistic is one of the most popular goodness-of-fit test statistics that is used to measure how well the distribution of a random sample $\left\{X_{1}, \ldots, X_{n}\right\}$ agrees with a theoretical distribution. It is defined as

$$
\begin{equation*}
D_{n}=\sup _{x}\left|F_{n}(x)-F(x)\right|, \tag{1}
\end{equation*}
$$

where $n$ is the sample size, $F_{n}(x)$ denotes the empirical (cumulative) distribution function (edf) of $\left\{X_{1}, \ldots, X_{n}\right\}$, and $F(x)$ denotes the cumulative distribution function (cdf) of a prespecified theoretical distribution under the null hypothesis $\left(H_{0}\right)$ that the sample $\left\{X_{1}, \ldots, X_{n}\right\}$
comes from $F(x)$.
Many authors have studied the distribution of $D_{n}$, i.e., its $\operatorname{cdf} \mathrm{P}\left(D_{n} \leq q \mid H_{0}\right), q \in[0,1]$ under the assumption that $F(x)$ is continuous. Kolmogorov (1933), Smirnov (1939), Feller (1948), Doob (1949), and Smirnov (1948) considered the limiting distribution of $D_{n}$. Massey (1951) showed that the exact distribution of $D_{n}$ is independent of $F(x)$ if $F(x)$ is continuous, and provided a table for exact critical levels of the K-S test corresponding to certain significance levels for sample sizes $n \leq 35$. Durbin (1968) studied the probability that the edf of an ordered sample of $n$ independent observations from the uniform $(0,1)$ distribution lies between two parallel straight lines. He also obtained the exact distribution of $D_{n}$ for $F(x)$ continuous, when the two parallel straight lines are $n y=a+n x$ and $n y=-a+n x$. Durbin (1968) also noted the important link between this probability and the double-boundary non-crossing probability for a Poisson process that is easier to compute. Epanechnikov (1968), Steck (1971), Noé (1972), Niederhausen (1981) obtained the exact distribution of $D_{n}$ when $F(x)$ is continuous, by studying the probability that the order statistics of $n$ uniform $[0,1]$ random variables all lie within an $n$-dimensional rectangle. For brevity, we will further refer to this probability as the rectangle probability for uniform order statistics. Numerically computing the distribution of $D_{n}$ when $F(x)$ is continuous is not easy and has been recently considered by Marsaglia, Tsang, and Wang (2003), Simard and L'Ecuyer (2011), Carvalho (2015), among others. Details related to these works and further references are provided in Section 3.3.

While performing K-S tests when $F(x)$ is continuous is widely applicable, there are many real-life applications, e.g., in biology, physics, engineering, finance, and insurance, in which fitting discrete or mixed distributions, i.e., with multiple jumps and continuous segments, to large samples of data is required. For example, Calabrese and Zenga (2010) modeled the bank loan recovery rates using mixed random variables, since empirical data suggest that loans are either not repaid at all (recovery rate $=0$ ), partially repaid (recovery rate between 0 and 1 ), or fully repaid (recovery rate $=1$ ). This leads to considering a mixed $\operatorname{cdf} F(x)$ with jumps at 0 and 1 and a continuous segment in between. It is important to accurately model bank loan recovery rates, because this is required by the Basel II solvency framework. Mixed distributions with multiple jumps arise also in reinsurance, in relation to fitting claim amount data in multi-layer excess-of-loss treaties. We consider such an example in Section 3.1. Furthermore, numerous risk modeling applications in (general) insurance, e.g., car insurance and catastrophe insurance, require fitting appropriate discrete distributions to claim numbers data. The need to fit discrete distributions to data naturally arises also in almost any field of research in science and economics. In all such cases, the underlying $\operatorname{cdf} F(x)$ has discontinuities at some points and it is important to be able to perform goodness-of-fit tests, such as the chi-squared test and the K-S test. As demonstrated by Pettitt and Stephens (1977), the K-S test for discrete distributions can have greater power than the chi-squared test. On the other hand, Noether (1963), Slakter (1965), and Walsh (1963) showed that conducting a discontinuous K-S test is more conservative than conducting a continuous K-S test in terms of accepting/rejecting the null hypothesis. Thus, as we illustrate in Section 3.1, a null hypothesis that a sample comes from a discontinuous distribution will be accepted more often if one uses the continuous K-S test, as opposed to using the discontinuous K-S test. It should also be noted that the sample size in many applications can be substantial. Therefore, it is important to accurately and efficiently perform K-S tests for $F(x)$ with discontinuities, when sample sizes are large. For the purpose, one needs to be able to efficiently and accurately compute probabilities of the type, $\mathrm{P}\left(D_{n} \geq q\right)$, known as the complementary cdf, for any values
of $n$ and $q, q \in[0,1]$. Addressing this problem is the main objective of this paper.
The distribution of the K-S test statistic $D_{n}$ in this more general case, when $F(x)$ may have jump discontinuities (including purely discrete $F(x)$ ), has been studied to a much lesser extent. In an early paper, Schmid (1958) found the limiting distribution of $D_{n}$ when $F(x)$ has countable number of jumps and is increasing between the jumps. Carnal (1962) has generalized Schmid (1958)'s formula by allowing constant segments between jumps. Conover (1972) provided an approach to finding the exact critical level for the one-sided K-S test statistics $D_{n}^{-}=\sup _{x}\left(F(x)-F_{n}(x)\right)$ and $D_{n}^{+}=\sup _{x}\left(F_{n}(x)-F(x)\right)$ for discontinuous $F(x)$. Approximated critical levels for the two-sided K-S test statistic $D_{n}$ were also provided. Gleser (1985) studied the exact power of two-sided K-S tests. He showed that existing algorithms designed for K-S tests with continuous $F(x)$ could be used (after some necessary adjustments) for K-S tests when $F(x)$ is discontinuous. Specifically, Gleser (1985) showed that the power of the K-S test when $F(x)$ has jump discontinuities could still be expressed as a rectangle probability with respect to uniform order statistics, but with modified non-linear boundaries. Therefore, the determinantal and recurrence formulae for the latter rectangle probability due to Steck (1971), Noé (1972) and Niederhausen (1981) could be applied in order to obtain the exact distribution of $D_{n}$ when $F(x)$ is discontinuous. However, implementing these results is computationally expensive, especially when the sample size is large, and may lead to numerical instabilities, as noted by some authors and also illustrated in Section 3.2.
In summary, computing the distribution of $D_{n}$ when $F(x)$ is discontinuous is even harder and much less explored than in the continuous case. To the best of our knowledge, no methods have been proposed in the literature to compute the exact distribution of $D_{n}$ when $F(x)$ is mixed. Looking at the statistical software literature, all major packages implement the K-S test only when $F(x)$ is continuous, see for example, the ks.test function of the package stats ( R Core Team 2016) and ks.test.imp of the package kolmim (Carvalho 2015) in R (R Core Team 2016), SPSS (IBM Corp. 2013), the ksmirnov function in Stata (StataCorp. 2013), the kstest function in MATLAB (The MathWorks Inc. 2012), the KolmogorovSmirnovTest function in Mathematica (Wolfram Research Inc. 2015).
There is one exception, Arnold and Emerson (2011) provide the R function ks.test as part of the package dgof that calculates exact $p$ values of the K-S test assuming $F(x)$ is purely discrete. In ks.test, a one-sided K-S $p$ value is calculated by combining the approaches of Conover (1972) and Niederhausen (1981), while two-sided K-S $p$ values are calculated by combining the approaches of Gleser (1985) and Niederhausen (1981). However, the ks.test function due to Arnold and Emerson (2011) only provides exact $p$ values for sample sizes less than or equal to 30 , since as noted by the authors, when the sample size is large, numerical instabilities may occur. In the latter case, Arnold and Emerson (2011) suggest using simulation to approximate $p$ values, which as we show in Section 3.2, is rather slow and inaccurate.
Our aim in this paper is two-fold. The first goal is to provide a fast and accurate method to compute $\mathrm{P}\left(D_{n} \geq q\right)$ when $F(x)$ is discontinuous (i.e., mixed or purely discrete), and thus obtain exact $p$ values of the K-S test for any (small or large) sample size $n$, and any $q \in[0,1]$, possibly close to 1 . Our second goal is to give the $\mathrm{C}++$ code and an R package KSgeneral, based on the $\mathrm{C}++$ code that implements this fast and accurate method, which we believe fills in the gap in the existing statistical software. As we will see, the proposed method is also applicable and highly competitive when $F(x)$ is continuous. The approach we take, described in Section 2.1, is to express $\mathrm{P}\left(D_{n} \geq q\right)$ as an appropriate rectangle probability for uniform order statistics, as noted by Gleser (1985), and to compute the latter probability using the

Fast Fourier Transform (FFT) method. FFT has been recently utilized by Moscovich and Nadler (2017) to calculate this rectangle probability when $F(x)$ is continuous. Furthermore, in Section 2.2, we provide a useful extension (cf., (15) and (20)) of Schmid (1958)'s asymptotic formula, relaxing his requirement for $F(x)$ to be increasing between jumps and thus allowing for any general mixed or purely discrete $F(x)$. Similar formula has been obtained by Carnal (1962), but the embedded implicit index structure makes its numerical implementation prohibitive. In Section 3, we illustrate the $\mathrm{C}++$ and the R implementation as the package KSgeneral of the proposed FFT-based method. In particular, in Section 3.1, we study its numerical properties based on some mixed (inflated) distributions and also illustrate the performance of the general asymptotic formula (15). We show in Section 3.2 that when $F(x)$ is purely discrete, our approach to computing $\mathrm{P}\left(D_{n} \geq q\right)$, based on FFT and the asymptotic formula (22), outperforms in terms of speed and accuracy the R function of Arnold and Emerson (2011), especially for large sample sizes. Finally, in Section 3.3, we consider the case of continuous $F(x)$ and compare with the state-of-the-art procedures of Simard and L'Ecuyer (2011) and Carvalho (2015).

## 2. Distribution of $D_{n}$ when $F(x)$ is discontinuous

It is well known that the distribution of $D_{n}$ does not depend on $F(x)$ when the latter cdf is continuous. To see this, note that

$$
\begin{align*}
D_{n} & =\sup _{-\infty<x<\infty}\left|F_{n}(x)-F(x)\right|=\sup _{0 \leq t \leq 1}\left|F_{n}\left(F^{-1}(t)\right)-F\left(F^{-1}(t)\right)\right|, \\
& =\sup _{0 \leq t \leq 1}\left|F_{n}\left(F^{-1}(t)\right)-t\right|=\sup _{0 \leq t \leq 1}\left|U_{n}(t)-t\right|, \tag{2}
\end{align*}
$$

where $F^{-1}(t) \equiv \inf \{x: F(x) \geq t\}, t \in[0,1]$, and $U_{n}(t)$ is the empirical cdf of the uniform random sample $\left\{U_{i}=F\left(X_{i}\right), i=1, \ldots, n\right\}$. In this section, we relax the assumption of continuity of $F(x)$ and assume that $F(x)$ is non-decreasing and right-continuous, with countable (possibly infinite) number of jumps. From the right-continuity of $F(x)$, it follows that $F\left(F^{-1}(t)\right) \geq t$ and $F^{-1}(F(x)) \leq x$ and hence, the distribution-free property, illustrated by (2) is no longer valid. Therefore, it becomes difficult to compute the exact and asymptotic distributions of $D_{n}$. This problem is addressed in the next two sections.

### 2.1. The exact distribution of $D_{n}$

Our approach to computing the exact distribution of $D_{n}$ is based on the following four major steps:

Step 1. It is not difficult to show (see Appendix A) that the complementary $\operatorname{cdf} \mathrm{P}\left(D_{n} \geq\right.$ $q), q \in[0,1]$, can be expressed in terms of a rectangle probability for the vector of $n$ uniform order statistics as

$$
\begin{equation*}
\mathrm{P}\left(D_{n} \geq q\right)=1-\mathrm{P}\left(A_{i} \leq U_{(i)} \leq B_{i}, 1 \leq i \leq n\right), \tag{3}
\end{equation*}
$$

where

$$
\begin{align*}
& A_{i}=\lim _{\epsilon \downarrow 0} F\left(\left(F^{-1}\left(\frac{i}{n}-q+\epsilon\right)\right)-\right) \\
& F(x-)=\lim _{z \uparrow x} F(z)=\mathrm{P}(X<x),  \tag{4}\\
& B_{i}=\lim _{\epsilon \downarrow 0} F\left(F^{-1}\left(\frac{i-1}{n}+q-\epsilon\right)\right), i=1,2, \ldots, n,
\end{align*}
$$

and where $U_{(i)}, i=1, \ldots, n$, are the order statistics of $n$ i.i.d. uniform $(0,1)$ random variables $U_{i}, i=1,2, \ldots, n$.

Step 2. Express the rectangle probability on the right hand side of (3) in terms of the double-boundary non-crossing probability with respect to the empirical process $\eta_{n}(t)=$ $n U_{n}(t)=\sum_{i=1}^{n} \mathbb{1}\left(U_{i} \leq t\right), 0 \leq t \leq 1$, where $U_{n}(t)$ is the edf of the sample $\left\{U_{1}, \ldots, U_{n}\right\}$. In particular, it can be directly verified that (3) can be rewritten as

$$
\begin{align*}
\mathrm{P}\left(D_{n} \geq q\right) & =1-\mathrm{P}\left(A_{i} \leq U_{(i)} \leq B_{i}, 1 \leq i \leq n\right) \\
& =1-\mathrm{P}\left(g(t) \leq \eta_{n}(t) \leq h(t), \forall 0 \leq t \leq 1\right) \tag{5}
\end{align*}
$$

where the upper and lower boundary functions $h(t), g(t)$ are defined as

$$
\begin{equation*}
h(t)=\sum_{i=1}^{n} \mathbb{1}_{\left(A_{i}<t\right)}, \quad g(t)=\sum_{i=1}^{n} \mathbb{1}_{\left(B_{i} \leq t\right)} . \tag{6}
\end{equation*}
$$

Let us note that $h(t)$ and $g(t)$ are correspondingly left and right continuous functions which equivalently satisfy the following conditions

$$
\begin{equation*}
\sup \{t \in[0,1]: h(t)<i\}=A_{i}, \text { and } \inf \{t \in[0,1]: g(t)>i-1\}=B_{i} \tag{7}
\end{equation*}
$$

with $A_{i}, B_{i}$ defined in $(4)^{1}$. The last equality in (5) is illustrated in Figure 1, where one can see that considering the rectangle probability with respect to the uniform order statistics, $\mathrm{P}\left(A_{i} \leq U_{(i)} \leq B_{i}, 1 \leq i \leq n\right)$ is equivalent to considering the non-exit probability, $\mathrm{P}\left(g(t) \leq \eta_{n}(t) \leq h(t), \forall 0 \leq t \leq 1\right)$.

Step 3. Use the fact that the process $\eta_{n}(t), t \in[0,1]$, has the same distribution as the conditional distribution of a Poisson process (PP) with intensity $n$, denoted by $\xi_{n}(t)$ : $[0,1] \mapsto\{0,1,2 \ldots\}$, given $\xi_{n}(1)=n$, (see e.g., Shorack and Wellner 2009, Chapter 8, Proposition 2.2). Therefore, the non-crossing probability in (5) can be re-expressed as

$$
\begin{align*}
& \mathrm{P}\left(g(t) \leq \eta_{n}(t) \leq h(t), \forall 0 \leq t \leq 1\right) \\
& =\mathrm{P}\left(g(t) \leq \xi_{n}(t) \leq h(t) \mid \xi_{n}(1)=n, \forall 0 \leq t \leq 1\right)  \tag{8}\\
& =\frac{\mathrm{P}\left(g(t) \leq \xi_{n}(t) \leq h(t) \text { and } \xi_{n}(1)=n, \forall 0 \leq t \leq 1\right)}{\mathrm{P}\left(\xi_{n}(1)=n\right)}=\frac{Q(1, n)}{e^{-n} n^{n} / n!}
\end{align*}
$$

where $\xi_{n}(1)$ follows a Poisson $(n)$ distribution and $Q(1, n)$ is defined as in (9). It is not difficult to see that in order to compute the non-crossing probability $\mathrm{P}(g(t) \leq$ $\xi_{n}(t) \leq h(t)$ and $\left.\xi_{n}(1)=n, \forall 0 \leq t \leq 1\right)$ on the right-hand-side of (8), defined on a continuum of times $t \in[0,1]$, it suffices to consider the events of non-crossing only over

[^0]

Figure 1: Illustration of the fact that the non-exit probability, $\mathrm{P}\left(A_{i} \leq U_{(i)} \leq B_{i}, 1 \leq i \leq n\right)$ is equivalent to the non-exit probability, $\mathrm{P}\left(g(t) \leq \eta_{n}(t) \leq h(t), \forall 0 \leq t \leq 1\right)$, where $g(t)$ and $h(t)$ are defined as in (6) using $F(x)$ given in (23) (cf., Example 2.8), with $n=5$.
some fixed times, $0=t_{0}<t_{1}<t_{2}<\ldots<t_{N}=1$, which are the ordered set of all distinct points in $\left\{1, A_{i}, B_{i}, i=1, \ldots, n\right\}$, where $A_{i}$ and $B_{i}$ are specified in (4) (and 7). Based on this discretization, similarly as done by Khmaladze and Shinjikashvili (2001) and Moscovich and Nadler (2017) in the continuous case, the non-crossing probability in (8) can be calculated by solving recursively an appropriate system of ChapmanKolmogorov forward equations ${ }^{2}$. In order to introduce these equations, for any $s \in[0,1]$ and $m \in\{0,1,2, \ldots$,$\} , let$

$$
\begin{equation*}
Q(s, m)=\mathrm{P}\left(g(t) \leq \xi_{n}(t) \leq h(t), \forall t \in[0, s] \text { and } \xi_{n}(s)=m\right), \tag{9}
\end{equation*}
$$

where $g(s) \leq m \leq h(s)$ and $Q(0,0)=\mathrm{P}(g(0) \leq 0 \leq h(0))=1$ by assumption. For any $j \in\{0,1, \ldots, N-1\}$ and any $m \in\{0,1,2, \ldots\}$, the Chapman-Kolmogorov equations are

$$
Q\left(t_{j+1}, m\right)=\left\{\begin{array}{l}
\sum_{g\left(t_{j}\right) \leq l \leq m} Q\left(t_{j}, l\right) \mathrm{P}\left(Y_{j}=m-l\right), \text { if } g\left(t_{j+1}\right) \leq m \leq h\left(t_{j+1}\right),  \tag{10}\\
0, \quad \text { otherwise },
\end{array}\right.
$$

where $Y_{j}$ denotes a Poisson random variable with parameter $n\left(t_{j+1}-t_{j}\right)$. The required non-crossing probability is obtained by computing $Q(1, n)$ following (10). This is illustrated by Figure 2, where $g(t)$ and $h(t)$ are obtained based on (6), with $F(x)$ defined in (23) as part of Example 2.8. The black dots illustrate the mesh of points $\left(t_{j+1}, m\right)$, $j=0,1, \ldots, 6, m=0,1,2, \ldots, 5$, at which non-crossing of the trajectory of $\xi_{n}(t)$ with the boundaries $g(t), h(t)$ may occur and the corresponding probabilities, $Q\left(t_{j+1}, m\right)$ need to be computed, following (10).

[^1]As shown by Khmaladze and Shinjikashvili (2001), the recurrent computation following (10) requires total running time of order at most $\mathcal{O}\left(n^{3}\right)$. In the next step we employ FFT in order to improve this rate.


Figure 2: Illustration of a trajectory of the Poisson process $\xi_{n}(t)$ staying in the corridor between the boundaries $h(t)$ and $g(t)$ defined as in (6) using $F(x)$ given in (23) (cf., Example 2.8). The black dots illustrate the mesh of points $\left(t_{j+1}, m\right), j=0,1, \ldots, 6, m=0,1,2, \ldots, 5$, at which non-crossing of the trajectory of $\xi_{n}(t)$ with the boundaries $g(t), h(t)$ may occur and the corresponding probabilities, $Q\left(t_{j+1}, m\right)$ need to be computed, following (10).

Step 4. Apply FFT to compute the truncated linear convolution of the vectors $\mathbf{Q}_{t_{j}}=$ $\left(Q\left(t_{j}, 0\right), Q\left(t_{j}, 1\right), \ldots, Q\left(t_{j}, n\right)\right)$ and $\boldsymbol{\pi}_{n\left(t_{j+1}-t_{j}\right)}=\left(\mathrm{P}\left(Y_{j}=0\right), \mathrm{P}\left(Y_{j}=1\right), \ldots, \mathrm{P}\left(Y_{j}=n\right)\right)$ in order to solve (10), as proposed by Moscovich and Nadler (2017), see Section 2 therein. As shown by these authors, the total running time of this method is of order at most $\mathcal{O}\left(n^{2} \log n\right)$, which is faster than $\mathcal{O}\left(n^{3}\right)$ especially for large $n$.

In summary, our approach to computing the exact $\mathrm{P}\left(D_{n} \geq q\right)$ when $F(x)$ is discontinuous is outlined in the following procedure.

## Procedure Exact-KS-FFT

(i) Specify a discontinuous cdf $F(x)$, a sample size $n$, and a quantile $q$.
(ii) As detailed in Step 1, compute $A_{i}$ and $B_{i}$ for $i=1, \ldots, n$, based on (4), where the limites are coded using a very small $\epsilon$, e.g., $\epsilon=10^{-10}$.
(iii) As detailed in Step 2, compute the upper and lower boundaries $g(t), h(t)$ using (6).
(iv) Following Steps 3 and 4, apply FFT to compute $Q(1, n)$ defined in (10). Hence, calculate the double-boundary non-crossing probability with respect to the PP
on the right-hand-side of (8) and respectively obtain the double-boundary noncrossing probability with respect to $\eta_{n}(t)$ on the left-hand-side of (8).
(v) Finally, compute the exact $\mathrm{P}\left(D_{n} \geq q\right)$ using (5) (cf., Steps 2 and 3).

Remark 2.1. Let us note that $\mathrm{P}\left(D_{n} \geq q\right), 0 \leq q \leq 1$, can directly be computed using (3) and (4), applying the determinantal formula for the rectangle probability in (3), due to Steck (1971), or the recurrence formula of Niederhausen (1981). However, such computations are slow, and may become unstable for sample sizes $n \geq 100$, as shown in Section 3.2, Example 3.5. We also note that $\mathrm{P}\left(D_{n} \geq q\right)$ is the $p$ value corresponding to a fixed critical level $q \in[0,1]$. Thus, if $q=d_{n}$, where $d_{n}$ is the value of the KS test statistic computed based on a sample $\left\{x_{1}, \ldots, x_{n}\right\}$, then the corresponding exact $p$ value, $\mathrm{P}\left(D_{n} \geq d_{n}\right)$ can be obtained through (3) and (4).
Remark 2.2. We have described the Procedure Exact-KS-FFT for computing the complementary cdf of the two-sided K-S statistic, $D_{n}$, defined in (1). It should be noted that by selecting the lower boundary $g(t) \equiv 0, \forall t$, and the upper boundary $h(t)$ as specified in (6) one can compute the complementary cdf for the one-sided K-S statistic $D_{n}^{+}=\sup _{x}\left(F_{n}(x)-F(x)\right)$. By selecting the upper boundary $h(t) \equiv n, \forall t$, and the lower boundary $g(t)$ as specified in (6), one can compute the complementary cdf for the one-sided K-S statistic $D_{n}^{-}=\sup _{x}\left(F(x)-F_{n}(x)\right)$ (see e.g., Gleser 1985). For the sake of consistency, in what follows, we illustrate the proposed FFT-based method for the two-sided version of the K-S statistic.
As noted and also demonstrated in Section 3, the proposed FFT-based method for computing exact $\mathrm{P}\left(D_{n} \geq q\right)$ is highly numerically efficient and could be easily applied to sample sizes $n$ up to hundreds of thousands (see also Moscovich and Nadler 2017). Nevertheless, it is still beneficial to know the asymptotic distribution of $D_{n}$ as $n \rightarrow \infty$, since as demonstrated in Section 3, it can be efficiently applied to approximate $\mathrm{P}\left(D_{n} \geq q\right)$ for large and even moderate sample sizes and hypothesized distributions with small number of jumps. The asymptotic distribution of $D_{n}$ will be considered in the next section.

### 2.2. The asymptotic distribution of $D_{n}$

Schmid (1958) has studied the asymptotic distribution of the form

$$
\begin{equation*}
\Phi(\lambda)=\lim _{n \rightarrow \infty} \mathrm{P}\left(D_{n}<\lambda n^{-\frac{1}{2}}\right)=\lim _{n \rightarrow \infty} \mathrm{P}\left(\sup _{-\infty<x<\infty}\left|F_{n}(x)-F(x)\right|<\lambda n^{-\frac{1}{2}}\right) \tag{11}
\end{equation*}
$$

where $n$ denotes the sample size, and $F(x)$ is a cdf with countable number of jumps $J$, at $x=x_{l}, l=1,2, \ldots, J$ and increasing continuous segments between the jumps. Let $F\left(x_{l}-\right)=$ $f_{2 l-1}, F\left(x_{l}\right)=f_{2 l}, l=1,2, \ldots, J$, with $f_{0}=0, f_{2 J+1} \equiv 1$, and $f_{2 l}<f_{2 l+1}, l=0, \ldots, J$. Under these assumptions on $F(x)$, Theorem 1 of Schmid (1958) states that

$$
\begin{align*}
& \Phi(\lambda)=\sum_{j_{1}=-\infty}^{\infty} \cdots \sum_{j_{J+1}=-\infty}^{\infty}(-1)^{j_{1}+\cdots+j_{J+1}} \\
& \times c \int_{-\lambda}^{\lambda} \cdots \int_{-\lambda}^{\lambda} \exp \left[-\frac{1}{2} \sum_{l=1}^{J} \frac{\left(z_{2 l}-z_{2 l-1}\right)^{2}}{f_{2 l}-f_{2 l-1}}-\frac{1}{2} \sum_{l=0}^{J} \frac{\left(z_{2 l+1}-(-1)^{j_{l+1}} z_{2 l}-2 \lambda j_{l+1}\right)^{2}}{f_{2 l+1}-f_{2 l}}\right] d z_{1} \cdots d z_{2 J} \tag{12}
\end{align*}
$$

where

$$
z_{0}=z_{2 J+1}=0, \text { and } c=(2 \pi)^{-J} \prod_{j=1}^{2 J+1}\left(f_{j}-f_{j-1}\right)^{-1 / 2}
$$

In view of (12), when the sample size $n$ is large, the limiting $\mathrm{P}\left(D_{n} \geq q\right)$ for mixed $F(x)$ can be calculated as

$$
\begin{equation*}
\lim _{n \rightarrow \infty} \mathrm{P}\left(D_{n} \geq q\right)=1-\Phi(\lambda) \tag{13}
\end{equation*}
$$

where $\Phi(\lambda)$ is expressed as in (12), and $\lambda=q n^{\frac{1}{2}}$. However, Schmid's formula cannot be applied if the condition $f_{2 l}<f_{2 l+1}, l=0, \ldots, J$ is not satisfied, since there will be division by 0 in the second denominator in (12). Therefore, (12) is not applicable if $F(x)$ has constant segments between (some of) the jumps, as is the case when $F(x)$ is purely discrete, or if $F(x)$ starts (ends) with a jump at 0 (at 1), as is the case for zero-inflated (mixed) distributions. Carnal (1962) has generalized Schmid (1958)'s formula to the case of arbitrary discontinuous $F(x)$ with finite number of jumps (cf., expression 5.1 therein). However, there is notational ambiguity (e.g., in the fourth summation in 5.1) and because the embedded index structure is rather implicit, it is not straightforward to implement formula (5.1) numerically. Therefore, in what follows, we will derive an alternative formula for $\Phi(\lambda)$, for any discontinuous $F(x)$ with finite number of jumps (see Proposition 2.3). The latter formula may look cumbersome, but as we will see, it is notationally explicit and therefore easier to implement numerically. In addition, we believe that the clearer and more intuitive proof of Proposition 2.3 will facilitate better understanding of the structure underlying (15). However, one should note that Formula (15) (respectively 20 and 22) is only practically implementable for small/moderate number of jumps, $J$, in the null distribution, as otherwise the multidimensional integration becomes infeasible.
It is not difficult to see that any jump structure in $F(x)$ can be represented through only two different types of continuous segments of $F(x)$ followed by jumps. The first one is a segment of $F(x)$ increasing on $\left[x_{l-1}, x_{l}-\right]$, i.e., $f_{2 l-2}<f_{2 l-1}$, followed by a jump at $x_{l}$, and the second one is a constant segment of $F(x)$ on $\left[x_{l-1}, x_{l}-\right]$, i.e., $f_{2 l-2}=f_{2 l-1}$, followed by a jump at $x_{l}$. We will refer to these two types of segments as "increasing-jump" segment and "flat-jump" segment, respectively.
We will use the notation $\nu_{1}, \nu_{2}, \ldots$ to denote the sizes of groups of consecutive increasing-jump segments, i.e., $\nu_{i}$ denotes the number of consecutive jumps, preceded by an increasing segment, in the $i^{\text {th }}$ group. Similarly, by $\omega_{k}, k=1,2, \ldots$, we denote the number of consecutive jumps preceded by a flat segment, in the $k^{t h}$ group. Without loss of generality, we assume that there are $m$ groups of increasing-jump and flat-jump segments, i.e., $\nu_{1}, \ldots, \nu_{m}$ and $\omega_{1}, \ldots, \omega_{m}$, and that these groups of jumps points, $x_{l}$, appear in the cdf in the following order:

$$
\begin{align*}
& \left\{x_{1}, \ldots, x_{\nu_{1}}, x_{\nu_{1}+1}, \ldots, x_{\nu_{1}+\omega_{1}}, x_{\nu_{1}+\omega_{1}+1}, \ldots, x_{\nu_{1}+\omega_{1}+\nu_{2}}, x_{\nu_{1}+\omega_{1}+\nu_{2}+1}, \ldots, x_{\nu_{1}+\omega_{1}+\nu_{2}+\omega_{2}}, \ldots\right. \\
& \left.x_{\nu_{1}+\omega_{1}+\cdots+\omega_{m-1}+1}, \ldots, x_{\nu_{1}+\omega_{1}+\cdots+\omega_{m-1}+\nu_{m}}, x_{\nu_{1}+\omega_{1}+\cdots+\omega_{m-1}+\nu_{m}+1}, \ldots, x_{\nu_{1}+\omega_{1}+\cdots+\omega_{m-1}+\nu_{m}+\omega_{m}}\right\} \tag{14}
\end{align*}
$$

where $\nu_{1}+\omega_{1}+\cdots+\nu_{m}+\omega_{m}=J$ is the total number of jumps in $F(x)$, and

$$
\nu_{1} \geq 0 ; \omega_{1} \geq 0 ; \nu_{1}+\omega_{1}>0 ; \nu_{l}>0,2 \leq l \leq m ; \omega_{l}>0,2 \leq l \leq m-1 ; \omega_{m} \geq 0 ; \nu_{m}+\omega_{m}>0 .
$$

It can be seen that (14) covers any possible order of the jumps of different type in $F(x)$ as illustrated on some examples below (see e.g., Corollary 2.6 and Example 2.8). Under these general assumptions on $F(x)$, in the following proposition we give a formula for $\Phi(\lambda)$ which generalizes (12).

Proposition 2.3. Assuming that a cdf $F(x)$ has the structure of jumps as in (14) and that $f_{2 J}=f_{2 J+1} \equiv 1$, we have

$$
\begin{equation*}
\Phi(\lambda)=\sum_{j_{1}=-\infty}^{\infty} \cdots \sum_{j_{v_{m}}=-\infty}^{\infty}\left((-1)^{j_{1}+\cdots+j_{v_{m}}}\right) c \int_{-\lambda}^{\lambda} \cdots \int_{-\lambda}^{\lambda} \exp \{\psi\} d z_{1} \cdots d z_{2 v_{m}+w_{m}-1} \tag{15}
\end{equation*}
$$

where

$$
\begin{align*}
c=\prod_{i=1}^{m} & \left(\prod_{l=1}^{\nu_{i}}\left(f_{2\left(v_{i-1}+w_{i-1}+l\right)-1}-f_{2\left(v_{i-1}+w_{i-1}+l\right)-2}\right)^{-1 / 2}\left(f_{2\left(v_{i-1}+w_{i-1}+l\right)}-f_{2\left(v_{i-1}+w_{i-1}+l\right)-1}\right)^{-1 / 2}\right) \\
& \times\left(\prod_{l=1}^{\omega_{i}}\left(f_{2\left(v_{i}+w_{i-1}+l\right)}-f_{2\left(v_{i}+w_{i-1}+l\right)-1}\right)^{-1 / 2}\right)(2 \pi)^{-\frac{2 v_{m}+w_{m}-1}{2}}, \tag{16}
\end{align*}
$$

and

$$
\begin{align*}
\psi=-\frac{1}{2} \sum_{i=1}^{m}\{ & \sum_{l=1}^{\nu_{i}}\left[\frac{\left(z_{2\left(v_{i-1}+l\right)+w_{i-1}}-z_{2\left(v_{i-1}+l\right)+w_{i-1}-1}\right)^{2}}{f_{2\left(v_{i-1}+w_{i-1}+l\right)}-f_{2\left(v_{i-1}+w_{i-1}+l\right)-1}}\right. \\
& \left.+\frac{\left(z_{2\left(v_{i-1}+l\right)+w_{i-1}-1}-(-1)^{j_{\left(v_{i-1}+l\right)}} z_{2\left(v_{i-1}+l\right)+w_{i-1}-2}-2 \lambda j_{\left(v_{i-1}+l\right)}\right)^{2}}{f_{2\left(v_{i-1}+w_{i-1}+l\right)-1}-f_{2\left(v_{i-1}+w_{i-1}+l\right)-2}}\right]  \tag{17}\\
& \left.+\sum_{l=1}^{\omega_{i}}\left[\frac{\left(z_{2 v_{i}+w_{i-1}+l}-z_{2 v_{i}+w_{i-1}+l-1}\right)^{2}}{f_{2\left(v_{i}+w_{i-1}+l\right)}-f_{2\left(v_{i}+w_{i-1}+l\right)-1}}\right]\right\}
\end{align*}
$$

with $\nu_{0}=\omega_{0}=0 ; v_{0}=w_{0}=0 ; v_{i}=\sum_{k=1}^{i} \nu_{k} ; w_{i}=\sum_{k=1}^{i} \omega_{k}, v_{m}+w_{m}=J$, and $z_{0}=$ $z_{2 v_{m}+w_{m}}=0$.

Proof: The reasoning in the proof follows that of Schmid (1958) with some necessary adjustments to account for the fact that $f_{2 l} \leq f_{2 l+1}$ as opposed to $f_{2 l}<f_{2 l+1}, l=0, \ldots, J$. So, here we only give details related to those parts of the proof which are affected by the relaxed assumption on $F(x)$. Thus, following Schmid (1958), page 1014, denote by $I$ the union of the closed intervals $\left[f_{2 l}, f_{2 l+1}\right], l=0, \ldots, J$ and let $M_{n}$ be the set of integers $j$ such that $j / n \in I$,

$$
M_{n}=\left\{k_{0}=0, \ldots, k_{1} ; k_{2}, k_{2}+1, \ldots, k_{3} ; \ldots ; k_{2 J}, k_{2 J}+1, \ldots, k_{2 J+1}=n\right\}
$$

where $k_{i}$ is such that $k_{i} / n \rightarrow f_{i}$, as $n \rightarrow \infty$. Note that if $f_{2 l}=f_{2 l+1}$ i.e., if we have a constant segment in the cdf $F(x)$, then $k_{2 l} \equiv k_{2 l+1}$ and both are included in the set $M_{n}$. Now, as demonstrated by Schmid (1958) (see expressions 20, 21 therein), the probability $\mathrm{P}_{0 n}:=\mathrm{P}\left(D_{n}<\lambda n^{-1 / 2}\right)$ in (11), can be calculated as

$$
\mathrm{P}_{0 n}=\frac{n!e^{n}}{n^{n}} R_{0 n}
$$

where

$$
\begin{equation*}
R_{i k_{2 l+1}}=\sum_{|j|<\lambda N^{1 / 2}} R_{j k_{2 l}} \mathrm{P}\left[\mathcal{D}_{i k_{2 l+1}} \mid \mathcal{D}_{i k_{2 l}}\right], \quad l=0, \ldots, J \tag{18}
\end{equation*}
$$

and

$$
\begin{equation*}
R_{i k_{2 l}}=\sum_{|j|<\lambda N^{1 / 2}} R_{j k_{2 l-1}} \frac{\left(k_{2 l}-k_{2 l-1}\right)^{i-j+k_{2 l}-k_{2 l-1}}}{\left(i-j+k_{2 l}-k_{2 l-1}\right)!e^{k_{2 l}-k_{2 l-1}}}, \quad l=0, \ldots, J, \tag{19}
\end{equation*}
$$

and $R_{00}=1, R_{i 0}=0$ for $i \neq 0$. Note that recursion (19) is related to the $l^{\text {th }}$ jump in $F(x)$, whereas recursion (18) is related to the continuous (increasing or flat) segment on $\left[x_{l}, x_{l+1}-\right]$ in $F(x)$. The events $\mathcal{D}_{i k}$ are specified in details in Schmid (1958) (see page 1016), but what is important here is to observe that when $k_{2 l}=k_{2 l+1}$ in $M_{n}, \mathrm{P}\left[\mathcal{D}_{i k_{2 l+1}} \mid \mathcal{D}_{i k_{2 l}}\right]=\mathbb{1}_{(i=j)}$. Thus, for a constant segment on $\left[x_{l}, x_{l+1}-\right]$ in $F(x)$, we have $R_{i k_{2 l+1}}=R_{i k_{2 l}}$ and so, recursion (18) is obsolete. Therefore, asymptotically, when $k_{2 l}=k_{2 l+1}$, we only need to consider the convergence of recursion (19) for a flat-jump segment in $F(x)$, whereas for increasing-jump segment, both recursions (18) and (19) generate terms in the resulting expression, in particular (16) and (17). Now, applying the asymptotic arguments outlined on page 1018 of Schmid (1958), one easily obtains formula (15).

Let us note that Proposition 2.3 does not cover the case when $f_{2 J}<f_{2 J+1} \equiv 1$. This case is addressed in the following proposition, which follows by similar reasoning.

Proposition 2.4. Assuming that a cdf $F(x)$ has the structure of jumps as in (14) and that $f_{2 J}<f_{2 J+1} \equiv 1, v_{m}+w_{m}=J$, we have
$\Phi(\lambda)=\sum_{j_{1}=-\infty}^{\infty} \ldots \sum_{j_{v_{m}}=-\infty}^{\infty} \sum_{j_{v_{m}+1}=-\infty}^{\infty}\left((-1)^{j_{1}+\cdots+j_{v_{m}}+j_{v_{m}+1}}\right) c^{\prime} \int_{-\lambda}^{\lambda} \cdots \int_{-\lambda}^{\lambda} \exp \left\{\psi^{\prime}\right\} d z_{1} \cdots d z_{2 v_{m}+w_{m}}$,
where

$$
\begin{equation*}
c^{\prime}=c\left(f_{2 J+1}-f_{2 J}\right)^{-1 / 2}(2 \pi)^{-1 / 2}, \quad \text { and } \quad \psi^{\prime}=\psi+\frac{\left(-(-1)^{j_{v_{m}+1}} z_{2 v_{m}+w_{m}}-2 \lambda j_{v_{m}+1}\right)^{2}}{f_{2 J+1}-f_{2 J}} \tag{21}
\end{equation*}
$$

with $c$ and $\psi$ in (21) defined in (16), (17), noting that $z_{2 v_{m}+w_{m}} \neq 0$.
Remark 2.5. Let us note that (12) is a special case of (20) when $m=1, \omega_{1} \equiv w_{1}=0, \nu_{1} \equiv$ $v_{1}=J$.

Corollary 2.6. When $F(x)$ is purely discrete with $J$ jumps, the limiting distribution $\Phi(\lambda)$ in (15) becomes

$$
\begin{equation*}
\Phi(\lambda)=(2 \pi)^{-\frac{J-1}{2}} \prod_{l=1}^{J}\left(f_{2 l}-f_{2 l-1}\right)^{-\frac{1}{2}} \int_{-\lambda}^{\lambda} \cdots \int_{-\lambda}^{\lambda} \exp \left[-\frac{1}{2}\left(\sum_{l=1}^{J} \frac{\left(z_{l}-z_{l-1}\right)^{2}}{f_{2 l}-f_{2 l-1}}\right)\right] d z_{1} \cdots d z_{J-1} \tag{22}
\end{equation*}
$$

where $z_{0}=z_{J}=0$.
Proof: Since the jump structure in this case includes only one group of flat-jump segments of size $J$, the first group of increasing-jump segments in (14) is empty, i.e., $m=1, \nu_{1} \equiv v_{1}=0$, $\omega_{1} \equiv w_{1}=J$, and by convention, $\prod_{l=1}^{\nu_{1}=0}(\cdot)=1, \sum_{l=1}^{\nu_{1}=0}(\cdot)=0$. Substituting these in (15), (16), and (17), we have

$$
c=(2 \pi)^{-\frac{J-1}{2}} \prod_{l=1}^{J}\left(f_{2 l}-f_{2 l-1}\right)^{-\frac{1}{2}}, \quad \psi=-\frac{1}{2}\left(\sum_{l=1}^{J} \frac{\left(z_{l}-z_{l-1}\right)^{2}}{f_{2 l}-f_{2 l-1}}\right)
$$

and (15) becomes (22).
Remark 2.7. It should be noted that (22) is the formula for the distribution of an $(J-$ 1) dimensional Brownian Bridge between $-\lambda$ and $\lambda$. The Brownian Bridge interpretation
has been used by Wood and Altavela (1978) to compute via Monte Carlo simulation the asymptotic distribution of $D_{n}$, without relating the interpretation to an explicit expression such as (22).
Next, we give an illustrative example on how to use the asymptotic distribution formula (15) given by Proposition 2.3, for mixed $F(x)$. Similarly, one can employ expressions (20) and (22) on appropriate specific examples.

Example 2.8. Consider a random variable $X$ with cdf

$$
F(x)=\left\{\begin{array}{l}
0 \text { if } \quad x<0,  \tag{23}\\
0.2+x \text { if } 0 \leq x<0.2 \\
0.5 \text { if } 0.2 \leq x<0.8 \\
x-0.1 \text { if } 0.8 \leq x<1, \\
1 \text { if } \quad x \geq 1
\end{array}\right.
$$

Clearly, $F(x)$ is a cdf with four jumps, i.e., $J=4$, at $x_{1}=0, x_{2}=0.2, x_{3}=0.8, x_{4}=1.0$, and $f_{0}=f_{1}=0, f_{2}=0.2, f_{3}=0.4, f_{4}=f_{5}=0.5, f_{6}=0.7, f_{7}=0.9, f_{8}=f_{9}=1$. Since the jump structure of $F(x)$ in (23) is flat-jump, increasing-jump, flat-jump, increasing-jump segments, the first set of increasing-jump segments and the last set of flat-jump segments in (14) should be omitted. Therefore, $m=3, \nu_{1}=0, \omega_{1}=1, \nu_{2}=1, \omega_{2}=1, \nu_{3}=1, \omega_{3}=0$, and $v_{0}=0, v_{1}=0, v_{2}=1, v_{3}=2, w_{0}=0, w_{1}=1, w_{2}=2, w_{3}=2$. Substituting these in (15), (16), and (17), we obtain

$$
\begin{equation*}
\Phi(\lambda)=\sum_{j_{1}=-\infty}^{\infty} \sum_{j_{2}=-\infty}^{\infty} c(-1)^{j_{1}+j_{2}} \int_{-\lambda}^{\lambda} \cdots \int_{-\lambda}^{\lambda} \exp \{\psi\} d z_{1} \cdots d z_{5}, \tag{24}
\end{equation*}
$$

where

$$
c=(2 \pi)^{-\frac{5}{2}}\left(f_{2}-f_{1}\right)^{-1 / 2}\left(f_{3}-f_{2}\right)^{-1 / 2}\left(f_{4}-f_{3}\right)^{-1 / 2}\left(f_{6}-f_{5}\right)^{-1 / 2}\left(f_{7}-f_{6}\right)^{-1 / 2}\left(f_{8}-f_{7}\right)^{-1 / 2}
$$

and
$\psi=-\frac{1}{2}\left(\frac{z_{1}^{2}}{f_{2}-f_{1}}+\frac{\left(z_{2}-(-1)^{j_{1}} z_{1}-2 \lambda j_{1}\right)^{2}}{f_{3}-f_{2}}+\frac{\left(z_{3}-z_{2}\right)^{2}}{f_{4}-f_{3}}+\frac{\left(z_{4}-z_{3}\right)^{2}}{f_{6}-f_{5}}+\frac{\left(z_{5}-(-1)^{j_{2}} z_{4}-2 \lambda j_{2}\right)^{2}}{f_{7}-f_{6}}+\frac{z_{5}^{2}}{f_{8}-f_{7}}\right)$.

## 3. Software implementation and numerical analysis

In this section, we introduce the $\mathrm{C}++$ and the R implementation of the proposed FFTbased method for computing $\mathrm{P}\left(D_{n} \geq q\right)$, described in Section 2.1 and study its numerical properties. In the sequel, we will refer to it as the Exact-KS-FFT method. The method is implemented in the R package KSgeneral which can be downloaded from the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/package=KSgeneral. In order to build the KSgeneral package from source, a C++ compiler is required. The latter is contained in the Windows program Rtools ( R Core Team 2016), or under MacOS in Xcode, downloadable from the App Store. The package KSgeneral uses Rcpp in R, and utilizes the $\mathrm{C}++$ code that efficiently computes $\mathrm{P}\left(D_{n} \geq q\right)$ using the Exact-KS-FFT method (see the Replication Material to this paper available online). Since the latter requires computation of

FFT, the FFTW3 library developed by Frigo and Johnson (2005) needs to be installed from http://www.fftw.org/index.html. It should be noted that both the Rtools and FFTW3 should be installed in the system PATH.
In this section, we also study the asymptotic formulae (15) and (22) given in Section 2.2, which have been implemented in Mathematica 10. For the purpose, in the next Sections 3.1 and 3.2, we compute the complementary cdf, $\mathrm{P}\left(D_{n} \geq q\right)$, for different values of $n$ and $q$, and also compute related $p$ values when $F(x)$ is mixed and discrete, respectively. Then, in Section 3.3 we consider $\mathrm{P}\left(D_{n}<q\right)$ and $\mathrm{P}\left(D_{n} \geq q\right)$ in the case of continuous $F(x)$. For the examples given in all three Sections 3.1, 3.2, 3.3 (and in the replication material), we give the lines of code that should be executed in $\mathrm{C}++$ or R using KSgeneral. Furthermore, in the case when $F(x)$ is mixed (cf., Section 3.1), we compare the exact probabilities $\mathrm{P}\left(D_{n} \geq q\right), q \in[0,1]$, obtained using the Exact-KS-FFT approach with those obtained using the asymptotic formula (15). In addition, when $F(x)$ is purely discrete (cf., Section 3.2), we also compare with the results of the Brownian Bridge simulation-based algorithm of Wood and Altavela (1978). When $F(x)$ is continuous, in Section 3.3, Appendix B, Appendix C, and Appendix D, we compare the accuracy and speed of the Exact-KS-FFT method to the results obtained from the R program of Carvalho (2015), and the C program due to Simard and L'Ecuyer (2011). The reported CPU times are obtained running the related $\mathrm{C}++$ code on a machine with an 2.5 GHz Intel Core i5 processor with 4GB RAM, running Mac OS X Yosemite.

### 3.1. Complementary cdf of $D_{n}$ when $F(x)$ is mixed

In order to illustrate the performance of the Exact-KS-FFT method of Section 2.1, we consider first the following example from excess-of-loss reinsurance.

Example 3.1. Consider an excess-of-loss reinsurance contract with a retention level $M$ and a limiting level $L$, where $0<M<L$ are positive constants. Under such a contract, given a loss amount random variable $X$ with a continuous $\operatorname{cdf} F_{X}(\cdot)$ on $[0,+\infty)$, the insurer and the reinsurer pay correspondingly the amounts $Z$ and $Y$, where

$$
Z=\left\{\begin{array}{l}
X \text { if } X \leq M, \\
M \text { if } M<X \leq L, \\
M+X-L \text { if } L<X,
\end{array} \text { and } \quad Y=\left\{\begin{array}{l}
0 \text { if } X \leq M, \\
X-M \text { if } M<X \leq L, \\
L-M \text { if } L<X .
\end{array}\right.\right.
$$

Clearly, both $Z$ and $Y$ are mixed random variables with correspondingly, one and two jumps in their cdfs. For illustrative purposes, assume that the cdf of $Y, F_{Y}(y)$ is of the form

$$
F_{Y}(y)=\left\{\begin{array}{l}
0 \text { if } y<0,  \tag{25}\\
1-0.5 e^{-y} \text { if } 0 \leq y<\log 2.5, \\
1 \text { if } y \geq \log 2.5
\end{array}\right.
$$

where $M=\log 2, L=\log 5, F_{X}(x)=1-e^{-x}$. Assuming $D_{n}$ in (1) is defined with respect to $F_{Y}(y)$, i.e., $F(x) \equiv F_{Y}(y)$ in (1), we have computed exact probabilities $\mathrm{P}\left(D_{n} \geq q\right)$, for different values of $n$ and $q$, applying the Exact-KS-FFT method and also, the asymptotic formula (15). In order to apply (15), one should note that $F_{Y}(y)$ has two jumps, (i.e., $J=2)$ at $x_{1}=0, x_{2}=\log 2.5$, and $f_{0}=f_{1}=0, f_{2}=0.5, f_{3}=0.8, f_{4}=f_{5}=1$. Since the jump structure of $F_{Y}(\cdot)$ in (25) is flat-jump, increasing-jump segments, the first set of increasing-jump segments and the last set of flat-jump segments in (14) should be omitted.

Therefore, one should apply formula (15) with $m=2, \nu_{1}=0, \omega_{1}=1, \nu_{2}=1, \omega_{2}=0$, and $v_{0}=0, v_{1}=0, v_{2}=1, w_{0}=0, w_{1}=1, w_{2}=1$.
The results for $\mathrm{P}\left(D_{n} \geq q\right)$ calculated using the proposed FFT-based method and the asymptotic formula (15), for different values of $n, q$, and respectively $\lambda=q n^{1 / 2}$, are shown in Table 1. For example, to obtain the probability $\mathrm{P}\left(D_{n} \geq q\right)$ using $\mathrm{C}++$, for $n=25, q=0.60$ as shown in the column Exact-KS-FFT of Table 1, according to step (i) of the Procedure Exact-KS-FFT, we first define the mixed cdf in (25) in the file "crossprob.cc" using the following code.

```
vector <double> MixDF (vector <double> obs){
    vector <double> observed = obs;
    set<double> s;
    for (int i = 0; i < obs.size(); ++i){
        s.insert(obs[i]);
    }
    obs.assign(s.begin(), s.end());
    vector <double> DF(obs.size());
    /* The distribution in the reinsurance example in (25) */
        for (int i = 0; i < obs.size(); ++i){
            if (obs[i] < 0.0){
                DF[i] = 0.0;
            }
            else if (obs[i] < log(2.5)){
                DF[i] = 1 - 0.5 * exp(-1.0 * obs[i]);
            }
            else
            {
                DF[i] = 1.0;
            }
        }
    return DF;
}
```

Also, since the mixed cdf in (25) has jumps at $y=0$ and $y=\log 2.5$, we need to specify this by inputting vector_input3 $=\{0.0, \log (2.5)\}$; to the int main() function in the file "crossprob.cc".
Next, we first run make in one of the command line tools (e.g., bash) to build the program for the Exact-KS-FFT method developed in this paper, based on the code provided by Moscovich and Nadler (2017). Then, in the command line tool, we run the following line ./bin/crossprob ecdf 25 Boundary_Crossing_Time.txt, where 25 is the input for the sample size. We will have the following screen prompts.

```
Please enter the distribution type: 1 for Continuous Distribution,
2 for Discontinuous Distributions:
```

We enter 2 since the cdf in (25) is not continuous.

Then, we can choose whether to calculate the K-S complementary cdf, $\mathrm{P}\left(D_{n} \geq q\right)$, or the $p$ value, $\mathrm{P}\left(D_{n} \geq d_{n}\right)$ corresponding to a value $d_{n}$ computed based on a user provided data sample.

```
Please enter the objective: 1 for K-S Complementary Distribution,
2 for P-Values:
```

Since we want to obtain the probability $\mathrm{P}\left(D_{n} \geq q\right)$, for $n=25, q=0.6$, we will enter 1 .

## 1

Here, we enter the sample size $n$ and the quantile $q$.
Please enter the sample size and quantile:

25
0.6

Probability: 0.0000000019082332
Time taken: 0.0000720000000000

Now, steps (ii), (iii), (iv) and (v) of the Procedure Exact-KS-FFT are performed. The result for $\mathrm{P}\left(D_{n} \geq q\right)$, for $n=25, q=0.60$, is $1.90823 \times 10^{-9}$ as shown in the column Exact-KS-FFT of Table 1. The corresponding computation time is also printed.

Remark 3.2. Note that the distribution of the K-S test statistic $D_{n}$ depends on the hypothesized distribution $F(x)$ when $F(x)$ is not continuous. Hence, to obtain $\mathrm{P}\left(D_{n} \geq q\right)$ for different mixed $F(x)$, the users should: 1) define the mixed cdf in the file "crossprob.cc" each time, and 2) in the file "crossprob.cc", define the vector containing points where $F(x)$ has jumps, vector_input3.
In order to compute $\mathrm{P}\left(D_{n} \geq q\right)$, when $F(x)$ is mixed using the R package KSgeneral, one needs to input mixed_ks_c_cdf(q, n, jump_points, Mixed_dist, ..., tol = 1e 10), where jump_points is a numeric vector of the $x$ coordinates of the jumps of $F(x)$, Mixed_dist specifies the mixed cdf $F(x)$, possibly followed by a list of parameters . . . specifying $F(x)$, and tol is the value of $\epsilon$ that is used to compute the values $A_{i}$ and $B_{i}, i=1, \ldots, n$, as detailed in Equations (4) in Step 1 of Section 2.1. By default, tol $=1 \mathrm{e}-10$. Note that a value NA or 0 will lead to an error. For instance, if one wants to use the R package KSgeneral to compute $\mathrm{P}\left(D_{n} \geq q\right)$, when $F(x)$ is the mixed cdf specified in Example 3.1 by Equation (25), with $n=25, q=0.1$, one needs to run the following code in order to obtain the corresponding result, as shown in Table 1 for $n=25, q=0.1$.

```
R> Mixed_cdf_example <- function(x)
+ {
+ result <- 0
+ if (x<0){
+ result <- 0
+ }
+ else if (x == 0){
```

```
+ result <- 0.5
+ }
+ else if (x < log(2.5)){
+ result <- 1 - 0.5 * exp(-x)
+ }
+ else{
+ result <- 1
+ }
+
+ return (result)
+ }
R> mixed_ks_c_cdf(0.1, 25, c(0, log(2.5)), Mixed_cdf_example)
```

```
[1] 0.76768489
```

From Table 1, one can first see that the Exact-KS-FFT method effectively computes $\mathrm{P}\left(D_{n} \geq\right.$ $q$ ) for small, medium and large sample sizes $n$ and various levels $q$, and gives exact probabilities in the range of $10^{-10}$ to 1 . It should be noted though that the method could become numerically unstable (producing negative values) when calculating probabilities of $10^{-11}$ or smaller. Similar issue has been observed by Simard and L'Ecuyer (2011) in the case of continuous $F(x)$. The column "Rel.err. (\%)" quantifies the relative error of the asymptotic value (for fixed $\lambda$ ) compared to the exact values in the fourth column (for various combinations of $n$ and $q$ resulting in the same $\lambda$ ). Furthermore, we see that when the sample size $n$ is large, results using formula (15) approximate closely the exact $\mathrm{P}\left(D_{n} \geq q\right)$, except when $\mathrm{P}\left(D_{n} \geq q\right)$ is nearly zero (when $\lambda=2,3$ in Table 1). Also, asymptotic Formula (15) gives better approximations to the exact values of $\mathrm{P}\left(D_{n} \geq q\right)$ as $q$ decreases, or equivalently, as $\mathrm{P}\left(D_{n} \geq q\right)$ increases. Moreover, as $\lambda$ decreases, values obtained from asymptotic formula (15) become better approximations to the exact $\mathrm{P}\left(D_{n} \geq q\right)$. Let us recall however that Formula (15) (respectively 20 and 22 ) is only practically implementable for small/moderate number of jumps, $J$, in the null distribution (which is the case with 25 illustrated in Table 1), as otherwise the multidimensional integration becomes infeasible.
In addition, as mentioned in Section 1, a null hypothesis that a sample comes from a discontinuous distribution will be accepted more often if one uses the continuous K-S test, as opposed to using the discontinuous K-S test. To illustrate this, assume that a random sample of size $n=25$ follows $F(x) \equiv F_{Y}(y)$ in (25) under $H_{0}$, and that the K-S test statistic for the sample is $d_{n}=0.25$. Then, the exact $p$ value of the test is $\mathrm{P}\left(D_{n} \geq 0.25 \mid H_{0}\right)=0.04496610$ and, with a significance level of $5 \%$, one should reject $H_{0}$. On the other hand, a $p$ value calculated using the complementary cdf of the distribution-free continuous K-S test statistic $D_{n}$ (i.e., when $F(x)$ in (1) is continuous) is $0.07360597>0.05$. Therefore, based on the latter $p$ value, one will not reject $H_{0}$. Similar situations are illustrated in Table 2 for larger sample sizes and different values of the test statistic $D_{n}$, where one can see that the differences between the values in the last two columns are higher than $58 \%$ (our experience shows that these are typically in the range $50 \%-65 \%$ ) and do not decrease with $n$. To the best of our knowledge, the K-S test in softwares such as R, SPSS, Stata, MATLAB, Mathematica is based on the distribution-free continuous K-S test statistic and the discontinuous (mixed and purely discrete) version is not implemented due to the lack of efficient and robust method such as the Exact-KS-FFT method we propose here.

| $\lambda$ | $n$ | $q$ | Exact-KS-FFT |  | Asympt. (15) | Rel.err. (\%) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3 | 25 | 0.60 | $1.90823 \times 10^{-9}$ | (0.000) | $1.72031 \times 10^{-8}$ | 801.52 |
|  | 100 | 0.30 | $9.49583 \times 10^{-9}$ | (0.000) | (5155.54) | 81.17 |
|  | 400 | 0.15 | $1.41586 \times 10^{-8}$ | (0.015) |  | 21.50 |
|  | 2500 | 0.06 | $1.62830 \times 10^{-8}$ | (0.202) |  | 5.65 |
|  | 10000 | 0.03 | $1.67952 \times 10^{-8}$ | (2.932) |  | 2.43 |
|  | 40000 | 0.015 | $1.69539 \times 10^{-8}$ | (59.86) |  | 1.49 |
|  | 90000 | 0.01 | $1.70076 \times 10^{-8}$ | (351.9) |  | 1.16 |
|  | 250000 | 0.006 | $1.74648 \times 10^{-8}$ | (3524) |  | 1.43 |
| 2 | 25 | 0.4 | $2.13209 \times 10^{-4}$ | (0.000) | $3.98459 \times 10^{-4}$ | 86.89 |
|  | 100 | 0.2 | $3.27304 \times 10^{-4}$ | (0.000) | (1.17) | 21.74 |
|  | 400 | 0.1 | $3.66979 \times 10^{-4}$ | (0.015) |  | 8.58 |
|  | 2500 | 0.04 | $3.86968 \times 10^{-4}$ | (0.195) |  | 2.97 |
|  | 10000 | 0.02 | $3.92912 \times 10^{-4}$ | (2.707) |  | 1.41 |
|  | 40000 | 0.01 | $3.95740 \times 10^{-4}$ | (57.14) |  | 0.69 |
|  | 90000 | $1 / 150$ | $3.96661 \times 10^{-4}$ | (341.3) |  | 0.45 |
|  | 250000 | 0.004 | $3.97390 \times 10^{-4}$ | (3465) |  | 0.27 |
| 1 | 25 | 0.2 | 0.151510006 | (0.000) | 0.174525238 | 15.19 |
|  | 100 | 0.1 | 0.164499986 | (0.000) | (0.73) | 6.09 |
|  | 400 | 0.05 | 0.169049900 | (0.015) |  | 3.24 |
|  | 2500 | 0.02 | 0.172221536 | (0.171) |  | 1.34 |
|  | 10000 | 0.01 | 0.173354312 | (2.511) |  | 0.68 |
|  | 40000 | 0.005 | 0.173934996 | (54.94) |  | 0.34 |
|  | 90000 | 1/300 | 0.174130680 | (330.3) |  | 0.23 |
|  | 250000 | 0.002 | 0.174287993 | (3423) |  | 0.14 |
| 0.5 | 25 | 0.1 | 0.767684886 | (0.000) | 0.801033877 | 4.35 |
|  | 100 | 0.05 | 0.782681427 | (0.000) | (5.63) | 2.35 |
|  | 400 | 0.025 | 0.790339869 | (0.015) |  | 1.35 |
|  | 2500 | 0.01 | 0.796406211 | (0.156) |  | 0.58 |
|  | 10000 | 0.005 | 0.798664879 | (2.441) |  | 0.30 |
|  | 40000 | 0.0025 | 0.799837547 | (54.27) |  | 0.15 |
|  | 90000 | 1/600 | 0.800234794 | (326.5) |  | 0.12 |
|  | 250000 | 0.001 | 0.800554870 | (3410) |  | 0.06 |
| 0.2 | 25 | 0.04 | 0.999798067 | (0.000) | 0.999961812 | 0.016 |
|  | 100 | 0.02 | 0.999888190 | (0.000) | (5.03) | 0.007 |
|  | 400 | 0.01 | 0.999925985 | (0.015) |  | 0.004 |
|  | 2500 | 0.004 | 0.999948507 | (0.156) |  | 0.001 |
|  | 10000 | 0.002 | 0.999955380 | (2.364) |  | 0.001 |
|  | 40000 | 0.001 | 0.999958655 | (53.62) |  | 0.000 |
|  | 90000 | 1/1500 | 0.999959721 | (324.4) |  | 0.000 |
|  | 250000 | 0.0004 | 0.999960564 | (3383) |  | 0.000 |
| 0.15 | 25 | 0.03 | 0.999998692 | (0.000) | 0.999999978 | 0.000 |
|  | 100 | 0.015 | 0.999999682 | (0.000) | (0.51) | 0.000 |
|  | 400 | 0.0075 | 0.999999905 | (0.015) |  | 0.000 |
|  | 2500 | 0.003 | 0.999999956 | (0.156) |  | 0.000 |
|  | 10000 | 0.0015 | 0.999999969 | (2.355) |  | 0.000 |
|  | 40000 | 0.00075 | 0.999999974 | (53.45) |  | 0.000 |
|  | 90000 | 0.0005 | 0.999999975 | (324.7) |  | 0.000 |
|  | 250000 | 0.0003 | 0.999999977 | (3372) |  | 0.000 |

Table 1: Exact and asymptotic values of $\mathrm{P}\left(D_{n} \geq q\right)$ obtained via the Exact-KS-FFT method and the asymptotic formula (15), when $\lambda=q n^{1 / 2}=3,2,1,0.5,0.2$ and 0.15 , respectively, when the underlying cdf $F(x)$ follows $F_{Y}(y)$ in (25). Numbers in () are run times in seconds.

| $n$ | $D_{n}=d_{n}$ | Discontinuous K-S $p$ values | Continuous K-S $p$ values |
| ---: | :--- | :---: | :---: |
| 25 | 0.25 | 0.04496610 | 0.07360597 |
| 100 | 0.13 | 0.03913182 | 0.06209234 |
| 400 | 0.065 | 0.04090172 | 0.06511744 |
| 2500 | 0.026 | 0.04200207 | 0.06690821 |
| 10000 | 0.013 | 0.04237475 | 0.06750119 |
| 40000 | 0.0065 | 0.04256212 | 0.06779695 |

Table 2: Discontinuous and continuous K-S $p$ values under null hypothesis $H_{0}: F(x) \equiv F_{Y}(y)$, obtained via the Exact-KS-FFT method.

Example 3.3. Another possible application of K-S tests on mixed distributions appears in testing the goodness-of-fit in zero-inflated or/and one-inflated models. Many real data contain zeros and ones, i.e., have masses at zero and one, and therefore zero- and one-inflated distributions need to be applied. For example, Ospina and Ferrari (2010) have used the zero-and-one-inflated beta distribution to model the proportion of inhabitants living within a 200 kilometer wide costal strip in 232 countries in the year 2000, denoted as $Y$. The data for years 1990, 2000 and 2010 are supplied by the Columbia University Centre for International Earth Science Information Network, see CIESIN (2012), and are available at http://sedac.ciesin. columbia.edu/data/set/nagdc-population-landscape-climate-estimates-v3. The zero-and-one-inflated beta distribution considered by Ospina and Ferrari (2010) is of the following form

$$
G_{Y}(y ; \alpha, \gamma, \mu, \phi)=\alpha \operatorname{Bernoulli}(y ; \gamma)+(1-\alpha) F(y ; \mu, \phi), \quad 0 \leq y \leq 1,
$$

where Bernoulli $(\cdot ; \gamma)$ denotes the cdf of a Bernoulli random variable with parameter $\gamma, 0<$ $\gamma<1$, and $F(\cdot ; \mu, \phi)$ denotes the cdf of a Beta random variable with parameters $\mu, 0<\mu<1$, and $\phi>0$. Hence, the zero-and-one-inflated distribution can be seen as a mixture of a (discrete) Bernoulli distribution and a (continuous) Beta distribution, with weights $\alpha$ and ( $1-\alpha$ ), respectively, $0<\alpha<1$.
According to Ospina and Ferrari (2010), the random variable $Y$ has the following distribution

$$
G_{Y}(y)=\left\{\begin{array}{l}
0 \text { if } y<0, \\
0.1141+0.4795 F_{Y}(y ; \mu, \phi) \text { if } 0 \leq y<1, \\
1 \text { if } y \geq 1,
\end{array}\right.
$$

where $F_{Y}(y ; \mu, \phi)$ has a density function

$$
f_{Y}(y ; \mu, \phi)=\frac{\Gamma(\phi)}{\Gamma(\mu \phi) \Gamma((1-\mu) \phi)} y^{\mu \phi-1}(1-y)^{(1-\mu) \phi-1},
$$

with $\mu$ and $\phi$ estimated as $\mu=0.6189, \phi=0.6615$ based on the population data in 2000 , and $\Gamma(\cdot)$ is the gamma function. Then, we can examine the goodness-of-fit of the distribution to the population data in 2010, denoted by $\tilde{Y}$, hypothesizing that $\tilde{Y}$ has the same distribution as $G_{Y}(y)$. Using (1) with $F(x) \equiv G_{Y}(y)$ and $F_{n}(x) \equiv G_{n}(y)$, where $G_{n}(y)$ is the edf of $\tilde{Y}$ computed from the population data in 2010, we obtain the K-S test statistic $d_{n}=0.09047$. Using the Exact-KS-FFT method, we compute a $p$ value of $0.03403<0.05$. Alternatively, applying the asymptotic formula (15), we obtain a $p$ value of 0.03641 , which is reasonably accurate, given the sample size of 232. Therefore, the K-S test indicates that the zero-and-oneinflated beta distribution estimated using population data in 2000 does not fit the population
data in 2010 at a significance level of $5 \%$, providing evidence for a change in the proportion of inhabitants in the decade.
In order to perform the one-sample two-sided K-S test, when $F(x)$ is mixed, one needs to input the code mixed_ks_test (x, jump_points, Mixed_dist, ..., tol = 1e - 10), where x is a numeric vector of data sample values, and where other arguments are defined similarly as in the function mixed_ks_c_cdf (). For instance, if one wants to use the R package KSgeneral to calculate the $p$ value for the K-S test, when $F(x)$ follows a zero-and-one-inflated beta distribution as in Example 3.3, with a sample of size $n=232$, one should run the following R code.

```
R> data("Population_Data")
R> mu <- 0.6189
R> phi <- 0.6615
R> a <- mu * phi
R> b <- (1 - mu) * phi
R> Mixed_cdf_example <- function(x)
+ {
+ result <- 0
+ if (x < 0){
+ result <- 0
+ }
+ else if (x == 0){
+ result <- 0.1141
+ }
+ else if (x < 1){
+ result <- 0.1141 + 0.4795 * pbeta(x, a, b)
+ }
+ else{
+ result <- 1
+ }
+
+ return (result)
+ }
R> ksgeneral::mixed_ks_test(Population_Data, c(0, 1), Mixed_cdf_example)
    One-sample Kolmogorov-Smirnov test
data: Population
D = 0.0904737, p-value = 0.034025
alternative hypothesis: two-sided
```

In the next section, assuming $F(x)$ is purely discrete, we apply the FFT-based methodology and the asymptotic formula (22) (cf., Corollary 2.6) to compute correspondingly, exact and approximate values of $\mathrm{P}\left(D_{n} \geq q\right)$.

### 3.2. Complementary cdf of $D_{n}$ when $F(x)$ is purely discrete

There is an abundance of real-life applications in which purely discrete distributions are used to model count data, such as: Number of claims to an insurance company, number of jumps in stock returns, number of trades on the stock exchange, number of manufacturing defects, number of diseased species and plants in biology and agricultural research, and many other count data applications. In all such cases, examining the goodness-of-fit of the model requires computing $p$ values or $\mathrm{P}\left(D_{n} \geq q\right)$ for various of $n$ and $q$. As an illustration, using the proposed FFT-based method, we will compute exact probabilities $\mathrm{P}\left(D_{n} \geq q\right)$ when the underlying $F(x)$ follows $\operatorname{Binomial}(r, \pi)$ distribution (see Example 3.4) and when it follows a discrete uniform distribution (see Example 3.5). In Example 3.4, we compare these Exact-KSFFT probabilities with approximate ones obtained using the asymptotic distribution of $D_{n}$, given by (22), and using the asymptotic Monte Carlo simulation-based method of Wood and Altavela (1978). In Example 3.5, we compare the Exact-KS-FFT results with those obtained using the R function ks.test of Arnold and Emerson (2011). The latter is a revised version of the same function from the recommended package stats.
Wood and Altavela (1978)'s approach utilizes the connection between the asymptotic distribution of $D_{n}$ and a multi-variate Brownian Bridge (cf., Remark 2.7), and they directly simulate the latter, thus avoiding the necessity to derive and evaluate an explicit expression such as (22). Following the Wood and Altavela (1978)'s method, one should simulate from the $(J-1)$-variate normal random vector $\left(Z_{1}, Z_{2}, \ldots, Z_{J-1}\right)$, where

$$
\begin{equation*}
\mathrm{E}\left(Z_{i}\right)=0, \quad \mathrm{E}\left(Z_{i}, Z_{k}\right)=\min \left(f_{2 i}, f_{2 k}\right)-f_{2 i} f_{2 k}, \quad i, k=1, \ldots, J-1, \tag{26}
\end{equation*}
$$

and estimate the probability in $\Phi(\lambda)$ in (11) as

$$
\frac{\sum_{i=1}^{N} \mathbb{1}_{\left\{\left(Z_{1}, Z_{2}, \ldots, Z_{J-1}\right) \in[-\lambda, \lambda]^{J-1}\right\}}}{N}
$$

where $N$ is the number of simulations, $\mathbb{1}_{\{\cdot\}}$ is an indicator function, and $[-\lambda, \lambda]^{J-1}$ is the $J-1$ dimensional hypercube. The authors further suggest a continuity correction for $\lambda$ in (11), as $\lambda=q n^{1 / 2}-0.5 n^{-1 / 2}$. In the remainder of this section, we will refer to this method as $W \& A(\mathrm{a})$ method and to its version without the continuity correction, as $W \& A(\mathrm{~b})$ method.

Example 3.4. Assume that $F(x)$ in (1) is $\operatorname{Binomial}(r, \pi)$ with $r=3,7,15$ (i.e., with $J=$ $r+1$ number of jumps), and $\pi=0.5$. In Tables 3,4 , and 5 , for different values of $n$, $q$, and respectively $\lambda=q n^{1 / 2}$, we give the exact $\mathrm{P}\left(D_{n} \geq q\right)$ obtained with the Exact-KSFFT method, and compare with the asymptotic probabilities obtained using (22) (combined with (13)), and using the Wood and Altavela (1978) simulation-based approach. We have coded both the $W \& A(\mathrm{a})$ and $W \& A(\mathrm{~b})$ versions in R as part of the KSgeneral R package and have simulated 1000000 realizations of the random vector $\left(Z_{1}, Z_{2}, \ldots, Z_{J-1}\right)$. As before, the numbers in parentheses show the computation (run) times, in seconds. Let us note that the multidimensional numerical integration in (22) becomes unstable as the number of jumps, $J=r+1$, in $F(x)$ increases, and so we only use $W \& A(\mathrm{a})$ and $W \& A(\mathrm{~b})$ to obtain approximate asymptotic probabilities in the case of $r=15$ and $\pi=0.5$ (see Table 5).
In order to compute $\mathrm{P}\left(D_{n} \geq q\right)$, when $F(x)$ is purely discrete using the R package KSgeneral, one needs to input disc_ks_c_cdf(q, $n, y, \ldots$, exact $=$ NULL, tol $=1 \mathrm{e}-08$, sim.size $=1 \mathrm{e}+06$, num.sim $=10$, where y specifies the purely discrete cdf $F(x)$, possibly followed by a list of parameters ... specifying $F(x)$, the input parameter exact is
a logical variable specifying whether one wants to compute exact values for $\mathrm{P}\left(D_{n} \geq q\right)$ using the FFT-based method, exact = TRUE or wants to compute the approximate values for $\mathrm{P}\left(D_{n} \geq q\right)$ using the simulation-based algorithm of Wood and Altavela (1978), in which case exact $=$ FALSE. When exact $=$ NULL and $\mathrm{n}<=100000$, the exact $\mathrm{P}\left(D_{n} \geq q\right)$ will be computed using the FFT-based method. The input parameter tol is the value of $\epsilon$ that is used to compute the values $A_{i}$ and $B_{i}, i=1, \ldots, n$, as detailed in Equations (4) in Step 1 of Section 2.1. By default, tol $=1 \mathrm{e}-08$. Note that a value of NA or 0 will lead to an error. The input parameter sim.size is the required number of simulated trajectories in order to produce one Monte Carlo estimate (one MC run) of the asymptotic $p$ value using the algorithm of Wood and Altavela (1978). By default, sim.size $=1 \mathrm{e}+06$. The input parameter num.sim is the number of MC runs, each producing one estimate (based on sim. size number of trajectories), which are then averaged in order to produce the final estimate for the asymptotic $p$ value. This is done in order to reduce the variance of the final estimate. By default, num.sim $=$ 10. For instance, if one wants to use the R package $\mathbf{K S g e n e r a l}$ to compute the exact value for $\mathrm{P}\left(D_{n} \geq q\right)$, when $F(x)$ follows a Binomial $(3,0.5)$ distribution as in Example 3.4, with $n=400, q=0.05$, one should run the following R code and obtain the corresponding result as shown in the column Exact-KS-FFT of Table 3.
$R>\operatorname{binom} 3$ <- stepfun $(c(0: 3), c(0, \operatorname{pbinom}(0: 3,3,0.5)))$
$R>$ disc_ks_c_cdf(0.05, 400, binom_3)
[1] 0.05611849
On the other hand, if one wants to use the simulation-based method of Wood and Altavela (1978) in order to approximate the asymptotic value for $\mathrm{P}\left(D_{n} \geq q\right)$, when $F(x)$ follows a $\operatorname{Binomial}(3,0.5)$ distribution, with $n=400, q=0.05$, one should use the W\&A (a) method, by running the following R code and obtain the corresponding result as shown in the column W\&A(a) of Table 3.

```
R> binom_3 <- stepfun(c(0 : 3), c(0, pbinom(0 : 3, 3, 0.5)))
R> disc_ks_c_cdf(0.05, 400, binom_3, exact = FALSE, tol = 1e-08,
+ sim.size = 1e+06, num.sim = 10)
```

[1] 0.0561864
Looking at Tables 3, 4, and 5 , one can see that the Exact-KS-FFT method effectively computes $\mathrm{P}\left(D_{n} \geq q\right)$ for small, medium and large sample sizes $n$ and various levels $q$, and gives exact probabilities in the range $10^{-12}$ to 1 . We also see that when the sample size $n$ is large, results using formula (22) approximate closely the exact $\mathrm{P}\left(D_{n} \geq q\right)$, except when $\mathrm{P}\left(D_{n} \geq q\right)$ is nearly zero (when $\lambda=2,3$ in Tables 3 and 4). Similarly to the mixed $F(x)$ case, asymptotic formula (22) gives better approximations to the exact values of $\mathrm{P}\left(D_{n} \geq q\right)$ as $q$ decreases, or equivalently, as $\mathrm{P}\left(D_{n} \geq q\right)$ increases. Moreover, as $\lambda$ decreases, values obtained from asymptotic formula (22) become better approximations to the exact $\mathrm{P}\left(D_{n} \geq q\right)$. One can further observe that asymptotic formula $(22)$ and $W \& A(b)$ method provide similar results. In particular, as the number of jumps in $F(x)$ increases, results obtained from these two methods almost coincide. In addition, when the number of jumps in $F(x)$ is small (in our case $J=4$ or 8 ), we see that values obtained from $W \& A(a)$ method provide more accurate approximations
to the exact probabilities. On the other hand, when the number of jumps in $F(x)$ is large (in our case $J=16$ ), values obtained from $W \& A(b)$ method give closer approximations. In comparison with the Exact-KS-FFT method, $W \& A(a)$ and $W \& A(b)$ deviate stronger from the exact probabilities for moderate values of $\lambda$, e.g., $\lambda=0.5,1$, and this is more pronounced for small sample sizes, see $n \leq 400$.
With regards to computation time, looking at Tables 3, 4, and 5, for fixed sample size $n$ and number of jumps $J$, as $\lambda$ decreases, the computation time for the Exact-KS-FFT method, $W \& A(a)$ method and $W \& A(b)$ method decreases. Furthermore, when the sample size $n$ and $q$ are fixed, as the number of jumps in $F(x)$, J, increases, the computation time for the Exact-KS-FFT method decreases, whereas the computation time for $W \& A(a)$ and $W \& A(b)$ methods increases. And, as expected, when the sample size $n$ increases, the Exact-KS-FFT method becomes more time-consuming.

Table 3: Exact and asymptotic values of $\mathrm{P}\left(D_{n} \geq q\right)$ obtained via the Exact-KS-FFT method, the asymptotic formula (22) and distribution. Numbers in () are run times in seconds.

| $\lambda$ | $n$ | $q$ | Exact-KS-FFT |  | Asympt. (22) | Rel.err. (\%) | W\&A(a) |  | Rel.err. (\%) | W\&A(b) | Rel.err. (\% \% |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3 | 25 | 0.60 | $2.74894 \times 10^{-10}$ | (0.000) | $\begin{aligned} & 6.9080877 \times 10^{-4} \\ & (32.43) \end{aligned}$ |  | 0 | (11.43) |  | $\begin{aligned} & \hline 0 \\ & (10.93) \end{aligned}$ |  |  |
|  | 400 | 0.15 | $2.06159 \times 10^{-9}$ | (0.015) |  |  | 0 | (10.92) |  |  |  |  |
|  | 10000 | 0.03 | $2.08064 \times 10^{-9}$ | (2.074) |  |  | 0 | (10.99) |  |  |  |  |
|  | 90000 | 0.01 | $1.91281 \times 10^{-9}$ | (259.6) |  |  | 0 | (10.94) |  |  |  |  |
| 2 | 25 | 0.40 | $4.20725 \times 10^{-5}$ | (0.000) | $\begin{aligned} & -6.6918504 \times 10^{-5} \\ & (34.01) \end{aligned}$ |  | $1.54867 \times 10^{-4}$ | (10.95) |  | $\begin{aligned} & 6.51 \times 10^{-5} \\ & (10.98) \end{aligned}$ | $\begin{aligned} & 17.770 \\ & 6.094 \\ & 3.640 \end{aligned}$ |  |
|  | 400 | 0.10 | $7.91684 \times 10^{-5}$ | (0.015) |  |  | $8.06000 \times 10^{-5}$ | (10.93) | -1.808 |  |  |  |
|  | 10000 | 0.02 | $6.93244 \times 10^{-5}$ | (1.840) |  |  | $6.81333 \times 10^{-5}$ | (10.94) | 1.718 |  |  |  |
|  | 90000 | 1/150 | $6.75595 \times 10^{-5}$ | (244.9) |  |  | $6.63333 \times 10^{-5}$ | (10.98) | 1.815 |  |  |  |
| 1 | 25 | 0.20 | 0.068266018 | (0.000) | $\begin{aligned} & 0.070168353 \\ & (35.39) \end{aligned}$ |  | 0.11542800 | (10.58) |  | $\begin{aligned} & 0.070035433 \\ & (10.75) \end{aligned}$ | $\begin{aligned} & 6.494 \\ & 1.266 \\ & 0.363 \\ & \hline \end{aligned}$ |  |
|  | 400 | 0.05 | 0.074899103 | (0.015) |  | 6.316 | 0.07965367 | (10.65) | -6.348 |  |  |  |
|  | 10000 | 0.01 | 0.070933439 | (1.606) |  | 1.079 | 0.07187410 | (10.71) | -1.326 |  |  |  |
|  | 90000 | 1/300 | 0.070290581 | (233.2) |  | 0.174 | 0.07064190 | (10.74) | -0.500 |  |  |  |
| 0.5 | 25 | 0.10 | 0.619487745 | (0.000) | $\begin{aligned} & 0.56366243 \\ & (45.96) \end{aligned}$ |  | 0.73754833 | (8.31) |  | $\begin{aligned} & 0.56379917 \\ & (8.96) \end{aligned}$ | 3.4180.6810.212 |  |
|  | 400 | 0.025 | 0.583754412 | (0.015) |  | 3.442 | 0.60684037 | (8.76) | -3.955 |  |  |  |
|  | 10000 | 0.005 | 0.567662656 | (1.481) |  | 0.705 | 0.57234977 | (8.93) | -0.826 |  |  |  |
|  | 90000 | 1/600 | 0.564996352 | (221.4) |  | 0.236 | 0.56664517 | (8.95) | -0.292 |  |  |  |
| 0.2 | 25 | 0.04 | 0.976334785 | (0.000) | $\begin{aligned} & 0.97713513 \\ & (89.49) \end{aligned}$ |  | 0.99938833 | (6.01) |  | $\begin{aligned} & 0.97713387 \\ & (6.80) \end{aligned}$ | $\begin{array}{ll}  & \\ 0.627 & \text { 〇 } \\ 0.137 & \text { O } \\ 0.046 & \text { O } \end{array}$ |  |
|  | 400 | 0.01 | 0.983298737 | (0.015) |  | 0.627 | 0.98756200 | (6.61) | -0.434 |  |  |  |
|  | 10000 | 0.002 | 0.978475846 | (1.404) |  | 0.137 | 0.97956150 | (6.73) | -0.111 |  |  |  |
|  | 90000 | 1/1500 | 0.977587940 | (216.5) |  | 0.046 | 0.97796337 | (6.78) | -0.038 |  |  |  |
| 0.1 | 25 | 0.020 | 0.999999999 | (0.000) | 0.99938850 |  | 1 | (4.97) |  | 0.99938833 |  |  |
|  | 400 | 0.005 | 0.999745396 | (0.015) | (11.75) | 0.036 | 0.99989767 | (5.72) | -0.015 | (6.00) |  |  |
|  | 10000 | 0.001 | 0.999472182 | (1.388) |  | 0.008 | 0.99955080 | (5.90) | -0.008 |  |  |  |
|  | 90000 | $1 / 3000$ | 0.999417006 | (214.6) |  | 0.003 | 0.99944667 | (5.97) | -0.003 |  |  |  |

Table 4: Exact and asymptotic values of $\mathrm{P}\left(D_{n} \geq q\right)$ obtained via the Exact-KS-FFT method, the asymptotic formula (22) and distribution. Numbers in () are run times in seconds.

| $\lambda$ | $n$ | $q$ | Exact-KS-FFT |  | W\&A(a) | Rel.err. (\%) | W\&A(b) | Rel.err. (\%) |  |
| :---: | ---: | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 3 | 25 | 0.60 | $4.08521 \times 10^{-10}$ | $(0.000)$ | 0 |  | $(21.75)$ |  | 0 |
|  |  |  |  |  |  |  |  |  |  |
|  | 400 | 0.15 | $2.32760 \times 10^{-9}$ | $(0.015)$ | 0 | $(21.78)$ |  | $(21.87)$ |  |
|  | 10000 | 0.03 | $2.21527 \times 10^{-9}$ | $(1.622)$ | 0 | $(21.79)$ |  |  |  |
|  | 90000 | 0.01 | $2.07134 \times 10^{-9}$ | $(186.3)$ | 0 | $(21.86)$ |  | $8.55 \times 10^{-5}$ |  |
| 2 | 25 | 0.40 | $6.62012 \times 10^{-5}$ | $(0.000)$ | $2.07367 \times 10^{-4}$ | $(21.60)$ |  | $(21.80)$ | 14.13 |
|  | 400 | 0.10 | $9.95661 \times 10^{-5}$ | $(0.015)$ | $1.06900 \times 10^{-4}$ | $(21.63)$ | -7.366 | 5.53 |  |
|  | 10000 | 0.02 | $9.05026 \times 10^{-5}$ | $(1.387)$ | $8.92667 \times 10^{-5}$ | $(21.70)$ | 1.366 |  | 3.78 |
|  | 90000 | $1 / 150$ | $8.88601 \times 10^{-5}$ | $(173.5)$ | $8.66333 \times 10^{-5}$ | $(21.76)$ | 2.506 |  | 0.08956207 |
| 1 | 25 | 0.20 | 0.089163050 | $(0.000)$ | 0.14505810 | $(20.65)$ |  | $(21.11)$ | 4.073 |
|  | 400 | 0.05 | 0.093364526 | $(0.015)$ | 0.10142243 | $(21.02)$ | -8.631 | 0.785 |  |
|  | 10000 | 0.01 | 0.090270911 | $(1.138)$ | 0.09184050 | $(21.13)$ | -1.739 |  | 0.178 |
|  | 90000 | $1 / 300$ | 0.089721687 | $(161.2)$ | 0.09031193 | $(21.10)$ | -0.658 |  |  |
| 0.5 | 25 | 0.10 | 0.715781619 | $(0.000)$ | 0.81817303 | $(15.09)$ |  | 0.65034803 |  |
|  | 400 | 0.025 | 0.659784355 | $(0.015)$ | 0.69382393 | $(16.38)$ | -5.159 | $(16.57)$ | 1.430 |
|  | 10000 | 0.005 | 0.652226764 | $(1.045)$ | 0.65902720 | $(16.49)$ | -1.043 |  | 0.288 |
|  | 90000 | $1 / 600$ | 0.650966899 | $(155.2)$ | 0.65323800 | $(16.54)$ | -0.349 | 0.095 |  |
| 0.2 | 25 | 0.04 | 0.992964654 | $(0.000)$ | 0.99996560 | $(11.24)$ |  | 0.99363783 |  |
|  | 400 | 0.01 | 0.994406641 | $(0.015)$ | 0.99733230 | $(12.10)$ | -0.294 | $(12.35)$ | 0.077 |
|  | 10000 | 0.002 | 0.993769635 | $(0.967)$ | 0.99457260 | $(12.24)$ | -0.081 |  | 0.013 |
|  | 90000 | $1 / 1500$ | 0.993672471 | $(151.6)$ | 0.99396553 | $(12.34)$ | -0.029 |  | 0.003 |
| 0.1 | 25 | 0.020 | 0.999999999 | $(0.000)$ | 1 |  | $(7.52)$ |  | 0.99996560 |
|  | 400 | 0.005 | 0.999974260 | $(0.015)$ | 0.99999750 | $(10.80)$ | -0.002 | $(11.22)$ | 0.001 |
|  | 10000 | 0.001 | 0.999966686 | $(0.951)$ | 0.99997897 | $(11.04)$ | -0.001 |  | 0.000 |
|  | 90000 | $1 / 3000$ | 0.999965549 | $(150.1)$ | 0.99997020 | $(11.14)$ | 0.000 |  | 0.000 |

Table 5: Exact and asymptotic values of $\mathrm{P}\left(D_{n} \geq q\right)$ obtained via the Exact-KS-FFT method and W\&A(a), W\&A(b) methods for $\lambda=q n^{1 / 2}=3,2,1,0.5,0.2$ and 0.1 , respectively, when the underlying cdf $F(x)$ follows Binomial ( $15,0.5$ ) distribution. Numbers in () are run times in seconds.

Example 3.5. Next, we consider another illustrative example where we compare the performance of the proposed Exact-KS-FFT method with the R function ks.test from the package dgof (Arnold and Emerson 2011). Hypothesizing that the underlying $F(x)$ in (1) follows a discrete uniform distribution on $[1,10]$, we have simulated random samples of size $n, 25 \leq n \leq 100000$, from the discrete uniform distribution on $[1,10]$ and have performed K-S tests on the simulated samples. In Table 6, we compute $p$ values corresponding to different values of the test statistic $D_{n}$ for the simulated samples of size $n$.

| $n$ | $D_{n}=d_{n}$ | Exact-KS-FFT |  | ks.test |  | ks.test(simulation) |  | W\&A(a) |  |
| ---: | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 25 | 0.2 | 0.1523 | $(0.0000)$ | 0.1523 | $(0.007)$ | 0.1465 | $(0.79)$ | 0.1910 | $(12.63)$ |
| 30 | 0.2 | 0.1133 | $(0.0000)$ | 0.1133 | $(0.007)$ | 0.125 | $(0.84)$ | 0.1194 | $(12.73)$ |
| 50 | 0.22 | 0.007164 | $(0.0000)$ | 0.007167 | $(0.014)$ | 0.007 | $(1.10)$ | 0.0078223 | $(13.36)$ |
| 100 | 0.2 | 0.00021 | $(0.0000)$ | NU |  | 0.0002 | $(4.10)$ | 0.0002277 | $(13.80)$ |
| 1000 | 0.02 | 0.5424 | $(0.0150)$ | NU |  | 0.5385 | $(8.35)$ | 0.5429 | $(11.08)$ |
| 5000 | 0.0094 | 0.4779 | $(0.2340)$ | NU |  | 0.509 | $(68.37)$ | 0.4781 | $(10.92)$ |
| 10000 | 0.0065 | 0.4975 | $(0.8890)$ | NU |  | 0.4985 | $(123.98)$ | 0.4977 | $(11.08)$ |
| 100000 | 0.00241 | 0.3343 | $(118.85)$ | NU |  | - | - | 0.3344 | $(11.80)$ |

Table 6: $p$ values obtained via the Exact-KS-FFT method, the R function ks.test, and $W \& A(a)$ method, when the underlying cdf $F(x)$ follows a discrete uniform distribution on $[1,10]$. Numbers in () are run times in seconds.

In order to perform the one-sample two-sided K-S test, when $F(x)$ is purely discrete, one needs to input the disc_ks_test ( $\mathrm{x}, \mathrm{y}, \ldots$, exact $=$ NULL, tol $=1 \mathrm{e}-08$, sim. size $=1 \mathrm{e}$ +06 , num.sim $=10$ ), where x is a numeric vector of data sample values, and where other arguments are defined similarly as in the function disc_ks_c_cdf(). For instance, in order to calculate the $p$ value for the K-S test, when $F(x)$ follows a Uniform $[1,10]$ distribution as in Example 3.5, with a sample size $n=1000$, one should run the following R code.

```
R> x4 <- sample(1 : 10, 1000, replace = TRUE)
R> disc_ks_test(x4, ecdf(1 : 10), exact = TRUE)
```

```
One-sample Kolmogorov-Smirnov test
```

data: x 4
D $=0.01, \mathrm{p}$-value $=0.97023$
alternative hypothesis: two-sided
As can be seen from Table 6, the Exact-KS-FFT method produces exact $p$ values for all sample sizes $25 \leq n \leq 100000$, whereas the function ks.test becomes numerically unstable (NU) for $n \geq 100$, as noted also by Arnold and Emerson (2011). To avoid instability, for large $n$ ks.test allows for estimating $p$ values via simulation, which may be insufficiently accurate or prohibitively time consuming, depending on the choice of the number of simulations (cf., the column ks.test(simulation) in Table 6 where the number of simulations is 2000). In contrast to the ks.test function, using the Exact-KS-FFT method, one obtains the exact $p$ value 0.3343 for sample size $n=100000$ in less than 2 minutes without any simulation. Moreover, note that the $p$ values in the column ks.test(simulation) in Table 6 are based on the suggested default number of 2000 replicates (i.e., obtained by implementing the $R$ code dgof::ks.test (x, ecdf(1 : 10), simulated.p.value $=$ TRUE,
$B=2000)$. Thus, each estimated $p$ value is likely to be different if we run another simulation and the relative error will also vary substantially, as we demonstrate in Table 7. To reduce the variation of the simulated $p$ values, one may wish to increase the number of simulations but that will increase even more the computation time and make it prohibitive even for $n>1000$. In addition, mainly due to the way it has been implemented, for $n>1000$ the number of simulations cannot be significantly increased, e.g., go beyond 4000 replicates.

| $F(x)$ | $n, q$ | Exact-KS-FFT | ks.test(simulation) | Rel.err. |
| :---: | :---: | :---: | :---: | :---: |
| Binomial(3, 0.5) | 10000, 0.02 | 0.0000659 | 0 | 100\% |
|  |  |  | 0.0005 | 658\% |
|  |  |  | 0 | 100\% |
| Binomial(3, 0.5) | 400, 0.05 | 0.05612 | 0.050 | 10.9\% |
|  |  |  | 0.061 | 8.7\% |
|  |  |  | 0.069 | 22.9\% |
| $\operatorname{Binomial}(7,0.5)$ | 10000, 0.01 | 0.07093 | 0.0760 | 7.14\% |
|  |  |  | 0.0895 | 26.2\% |
|  |  |  | 0.0745 | 5.03\% |
| $\operatorname{Binomial}(7,0.5)$ | 400, 0.05 | 0.07490 | 0.0825 | 10.1\% |
|  |  |  | 0.0910 | 21.5\% |
|  |  |  | 0.0885 | 18.2\% |

Table 7: Differences between the exact and simulated values of $\mathrm{P}\left(D_{n} \geq q\right)$ obtained via the Exact-KS-FFT method and the R function ks.test, respectively, for certain $n>100$ and $q$, when the underlying $F(x)$ follows $\operatorname{Binomial}(3,0.5)$ or $\operatorname{Binomial}(7,0.5)$ distribution.

As can be seen from Table 7 (which extends Tables 3 and 4) and as also supported by many additional calculations we have run, even for $n \leq 10000$ the accuracy of the R function dgof: :ks.test may vary substantially for $p$ values in the (rather important) range $(0,0.1)$.
For small, moderate to large sample sizes (e.g., $25 \leq n \leq 10000$ ), looking at the column W\&A(a) of Table 6, one can see that the alternative MC simulation-based $W \& A(a)$ method produces less accurate results and can be significantly slower than the Exact-KS-FFT method. $W \& A(a)$ performs better in terms of the trade-off between accuracy and speed for very large sample sizes, e.g., $n=100000$.

To conclude, the proposed method outperforms the R function ks.test from the package dgof in all of the tested cases. When the number of jumps in the underlying $F(x)$ is small, the asymptotic $p$ value obtained from (22) may not be a good estimate unless sample sizes are very large (e.g., $\geq 40000$ ). Whereas when the number of jumps in $F(x)$ is large, one may use the limiting $p$ values to approximate the exact ones for large samples. In the next section, we turn our attention to the case of K-S tests with continuous null distributions, which has been widely studied in the literature and for which very efficient numerical procedures have been recently developed.

## 3.3. (Complementary)cdf of $D_{n}$ when $F(x)$ is continuous

Our purpose in this section is to illustrate the numerical performance of the proposed FFTbased approach of Section 2.1 and compare it with the state-of-the-art routines of Simard and L'Ecuyer (2011) and Carvalho (2015) developed especially for the case when the underlying
cdf, $F(x)$, is strictly continuous. These authors have summarized and enhanced further the most accurate and efficient methods for computing the distribution of $D_{n}$ for $F(x)$ continuous, developed earlier in a series of papers e.g., by Durbin (1968), Durbin (1973), Pomeranz (1974), Ruben and Gambino (1982), Marsaglia et al. (2003) and Brown and Harvey (2008). For comparison and further details on the implementations of these methods in various statistical softwares, we refer to Simard and L'Ecuyer (2011) and Brown and Harvey (2007). In their recent paper, Simard and L'Ecuyer (2011) have combined into one state-of-the-art program different exact methods to compute the distribution of $D_{n}$ for different combinations of $n$ and $q$, based on the relative efficiency and accuracy of the methods. Moreover, for certain combinations of $n$ and $q$, where the implementations of the exact methods break down (due to cancellation errors, loss of precision and/or prohibitive running time), e.g., for very large $n$ or when the cdf of $D_{n}$ is close to one, Simard and L'Ecuyer (2011) incorporate in their program various asymptotic formulae for the limiting distribution of $D_{n}$. We refer the reader to Section 4 in Simard and L'Ecuyer (2011) for further details. More recently, Carvalho (2015), by avoiding the direct calculation of powers of matrices as required by the approach of Durbin (1973), developed the R package kolmim with function pkolmim that produces results with similar accuracy as those obtained by the routine of Marsaglia et al. (2003), but much faster. However, the related R function becomes too slow when $n>10000$ as the running time is proportional to $n^{3}$ on average. We will show this in Appendix D.
Let us reemphasize that the proposed FFT-based method developed in Section 2.1 is general and thus, applicable also for the case when $F(x)$ is continuous. Hypothesizing on a continuous distribution $F(x)$ leads to certain simplifications. In particular, (3) of Step 1 simplifies to

$$
\begin{equation*}
\mathrm{P}\left(D_{n} \geq q\right)=1-\mathrm{P}\left(\frac{i}{n}-q \leq U_{(i)} \leq \frac{i-1}{n}+q, 1 \leq i \leq n\right), \tag{27}
\end{equation*}
$$

which confirms that the distribution of $D_{n}$ no longer depends on $F(x)$. Also, (5) of Step 2 simplifies to (27) since the boundaries in (6) become $g(t)=n t-n q$ and $h(t)=n t+n q$, $q \geq 0$ as shown by Durbin (1968). This special case of the proposed FFT-based method has been considered by Moscovich and Nadler (2017) in the general context of computing the probability of non-crossing an upper and lower boundaries by a PP.
Similarly to Simard and L'Ecuyer (2011) (see Sections 4 and 5 therein), we consider three regions of $n$, (i) $n \leq 140$, (ii) $140<n \leq 10^{5}$, and (iii) $n>10^{5}$, forming various sub-regions with respect to $q$, as specified in Appendix B and Appendix C. Within these sub-regions Simard and L'Ecuyer (2011) use different methods to compute the distribution of $D_{n}$. We have performed a thorough numerical comparison across these regions with details given in Appendix B and Appendix C, and can report that, with only a few exceptions, the Exact-KS-FFT method returns values that are of at least the same precision as those obtained from the R or C program.

## 4. Conclusions

We have provided a fast and accurate method to compute $\mathrm{P}\left(D_{n} \geq q\right)$ when $F(x)$ is arbitrary, discontinuous (i.e., mixed or purely discrete) or continuous. The approach we take is to express $\mathrm{P}\left(D_{n} \geq q\right)$ as an appropriate rectangle probability for uniform order statistics and to compute the latter probability using the FFT method. We demonstrate that the proposed

Exact-KS-FFT method is numerically efficient and robust when hypothesizing on either discontinuous or continuous $F(x)$. In particular, when $F(x)$ is purely discrete the proposed method outperforms in terms of speed and accuracy the R function of Arnold and Emerson (2011), especially for large sample sizes. Furthermore, in the case of continuous $F(x)$ the Exact-KS-FFT method represents a viable alternative to the state-of-the-art methods of Carvalho (2015) and Simard and L'Ecuyer (2011) as it returns values that are of at least the same precision. In the case when $F(x)$ is mixed, to the best of our knowledge no alternative methods have been proposed in the literature to compute the exact distribution of $D_{n}$.
In this paper, we have also derived a useful extension of Schmid (1958)'s asymptotic formula, relaxing his requirement for $F(x)$ to be increasing between jumps and thus allowing for any general mixed or purely discrete $F(x)$. As demonstrated numerically, the extended asymptotic formula provides reasonably close approximations to the exact values of $\mathrm{P}\left(D_{n} \geq q\right)$ and can successfully be used for small to moderate number of jumps in $F(x)$ and large sample sizes.
As part of a separate ongoing research, we have also demonstrated that the FFT-based method can be successfully applied to compute the complementary cdf of the weighted version of the K-S test statistic

$$
K_{n}=\sup _{x} \sqrt{n}\left|F_{n}(x)-F(x)\right| \sqrt{\psi[F(x)]},
$$

where $\psi(t) \geq 0, \forall t \in[0,1]$ is a weight function, first considered by Anderson and Darling (1952). The result of this additional research will appear elsewhere. Finally, as noted in Remark 4.3, the complementary cdfs $\mathrm{P}\left(D_{n} \geq q\right)$ and $\mathrm{P}\left(D_{n}>q\right)$ are non-increasing functions with jumps at some values of $q$. Characterizing in detail the distribution of $D_{n}$, in particular the points of discontinuity, in relation to $F(x)$ is also a subject of ongoing research.

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## A. Expressing $\mathrm{P}\left(D_{n}>q\right)$ and $\mathrm{P}\left(D_{n} \geq q\right)$ in terms of a rectangle probability with respect to the uniform order statistics

Lemma 4.1. The following holds true

$$
\mathrm{P}\left(D_{n}>q\right)=1-\mathrm{P}\left(\tilde{A}_{i} \leq U_{(i)} \leq \tilde{B}_{i}, 1 \leq i \leq n\right),
$$

where $\tilde{A}_{i}=F\left(\left(F^{-1}\left(\frac{i}{n}-q\right)\right)-\right)$ and $\tilde{B}_{i}=F\left(F^{-1}\left(\left(\frac{i-1}{n}+q\right)+\right)\right)$ and $F^{-1}(y+)=\lim _{\epsilon \downarrow 0} F^{-1}(y+$ $\epsilon)$.

Proof: We have

$$
\begin{aligned}
\mathrm{P}\left(D_{n}>q\right) & =\mathrm{P}\left(\sup _{-\infty<x<\infty}\left|F_{n}(x)-F(x)\right|>q\right) \\
& =1-\mathrm{P}\left(\sup _{-\infty<x<\infty}\left|F_{n}(x)-F(x)\right| \leq q\right) \\
& =1-\mathrm{P}\left(\left|F_{n}(x)-F(x)\right| \leq q, \text { for all } x\right) \\
& =1-\mathrm{P}\left(-q \leq F_{n}(x)-F(x) \leq q, \text { for all } x\right) \\
& =1-\mathrm{P}\left(F(x)-q \leq F_{n}(x) \leq F(x)+q, \text { for all } x\right) \\
& =1-\mathrm{P}\left(F\left(X_{(i)}-\right)-q \leq F_{n}\left(X_{(i-1)}\right) \text { and } F_{n}\left(X_{(i)}\right) \leq F\left(X_{(i)}\right)+q, \text { for } 1 \leq i \leq n\right) \\
& =1-\mathrm{P}\left(F\left(X_{(i)}-\right) \leq \frac{i-1}{n}+q \text { and } \frac{i}{n}-q \leq F\left(X_{(i)}\right), \text { for } 1 \leq i \leq n\right) \\
& =\mathrm{P}\left(F\left(X_{(i)}-\right)>\frac{i-1}{n}+q \text { or } \frac{i}{n}-q>F\left(X_{(i)}\right), \text { for some } 1 \leq i \leq n\right) \\
& =\mathrm{P}\left(F^{-1}\left(\left(\frac{i-1}{n}+q\right)+\right)<X_{(i)} \text { or } F^{-1}\left(\frac{i}{n}-q\right)>X_{(i)} \text { for some } 1 \leq i \leq n\right),
\end{aligned}
$$

where in the last equality we have applied that $u<F(x-)$ if and only if $F^{-1}(u+)<x$ and that $x<F^{-1}(u)$ if and only if $F(x)<u$ (see e.g., Lemma 1 (iii) and (v) of Gleser (1985)). Therefore, we now have

$$
\begin{align*}
\mathrm{P}\left(D_{n}>q\right) & =1-\mathrm{P}\left(F^{-1}\left(\frac{i}{n}-q\right) \leq X_{(i)} \leq F^{-1}\left(\left(\frac{i-1}{n}+q\right)+\right) \text { for } 1 \leq i \leq n\right) \\
& =1-\mathrm{P}\left(F\left(\left(F^{-1}\left(\frac{i}{n}-q\right)\right)-\right) \leq U_{(i)} \leq F\left(F^{-1}\left(\left(\frac{i-1}{n}+q\right)+\right)\right) \text { for } 1 \leq i \leq n\right) \tag{28}
\end{align*}
$$

where in the last equality we have applied Lemma 1 of Dimitrova, Ignatov, and Kaishev (2017). The statement now follows noting that one can rewrite the last equality in terms of $\tilde{A}_{i}$ and $\tilde{B}_{i}$.

Remark 4.2. The fact that the non-crossing probability

$$
\begin{aligned}
& \mathrm{P}\left(F(x)-q \leq F_{n}(x) \leq F(x)+q, \text { for all } x\right) \\
& =\mathrm{P}\left(F^{-1}\left(\frac{i}{n}-q\right) \leq X_{(i)} \leq F^{-1}\left(\left(\frac{i-1}{n}+q\right)+\right) \text { for } 1 \leq i \leq n\right)
\end{aligned}
$$

shown in the proof of Lemma 4.1 is illustrated in Figure 3 with $F(x)$ (the green piecewise linear function) defined in (23) (cf., Example 2.8), for $n=5$.

Remark 4.3. The statement of Lemma 4.1 holds true also for $\mathrm{P}\left(D_{n} \geq q\right)$, as stated in (3), with $A_{i}$ and $B_{i}$ defined as in (4). The proof is similar but more involved than that of Lemma 4.1 and is therefore omitted. It should also be noted that the complementary cdfs $\mathrm{P}\left(D_{n} \geq q\right)$ and $\mathrm{P}\left(D_{n}>q\right)$ are non-increasing functions with jumps at some values of $q$. In fact, these two functions coincide, except at the jumps where $\mathrm{P}\left(D_{n} \geq q\right)$ is left-continuous and $\mathrm{P}\left(D_{n}>q\right)$ is right-continuous. This is a consequence of the fact that the pairs $A_{i}, B_{i}$ and $\tilde{A}_{i}, \tilde{B}_{i}$ coincide except at their points of discontinuity, where $A_{i}, B_{i}$ are correspondingly right- and left- continuous, whereas $\tilde{A}_{i}, \tilde{B}_{i}$ are correspondingly left- and right- continuous.

Remark 4.4. Let us note that the result of Lemma 4.1 coincides with Theorem 1 of Gleser (1985).


Figure 3: Illustration of the equivalence of $\mathrm{P}\left(F(x)-q \leq F_{n}(x) \leq F(x)+q\right.$, for all $\left.x\right)$ to $\mathrm{P}\left(F^{-1}\left(\frac{i}{n}-q\right) \leq X_{(i)} \leq F^{-1}\left(\left(\frac{i-1}{n}+q\right)+\right)\right.$ for $\left.1 \leq i \leq n\right)$ (cf., Remark 4.2), for $F(x)$ defined as in (23) with $n=5$.

## B. Computing the cdf of $D_{n}$ when $F(x)$ is continuous: numerical analysis and comparisons

In this appendix, we compute the values of the $\operatorname{cdf} \mathrm{P}\left(D_{n} \leq q\right)$ for different $n$ and $q$ using the Exact-KS-FFT method and compare the results to those obtained with the $C$ program due to Simard and L'Ecuyer (2011) and R function pkolmim from the package kolmim by Carvalho (2015), which is claimed to be highly efficient and precise. Hence, we calculate an absolute error as the absolute difference between our results and the $R$ outputs, from which we can infer the number of decimal digits of precision of our results.
In order to compute $\mathrm{P}\left(D_{n} \leq q\right)$, when $F(x)$ is continuous using the R package KSgeneral, one needs to input cont_ks_cdf (q, n). For example, in order to compute the value for $\mathrm{P}\left(D_{n} \leq q\right)$, when $F(x)$ is continuous, for $n=40, n q^{2}=0.76$, one should run the following R code and obtain the corresponding result as shown in Table 10 for $n=40$ in the column Exact-KS-FFT.
$R>$ cont_ks_cdf(sqrt $(0.76 / 40), 40)$
[1] 0.6032371

Simard and L'Ecuyer (2011) consider the following regions: 1) $n \leq 140$ and $q \leq 1 / n$; 2) $n \leq 140$ and $q \geq 1-1 / n$; 3) $n \leq 140$ and $1 / n<n q^{2}<0.754693$; 4) $n \leq 140$ and $0.754693 \leq$ $n q^{2}<4$; 5) $n \leq 140$ and $4 \leq n q^{2}<18$; 6) $n \leq 140$ and $n q^{2} \geq 18$; 7) $140<n \leq 10^{5}$ and $n q^{3 / 2}<1.4$; 8) $140<n \leq 10^{5}$ and $n q^{3 / 2} \geq 1.4$; and 9) $n>10^{5}$ where they use different methods to compute the distribution of $D_{n}$ (cf., Simard and L'Ecuyer 2011, Section 4).
Following the segmentation of regions, we have computed the distribution of $D_{n}$ with the proposed FFT-based method and can report that for regions 1), 2), 3), 4), 7), our approach gives results that are of at least the same precision as those obtained from the R or C program. In regions 5) and 6), when $n \leq 140$ and $n q^{2}>12$, our approach may be unsuitable due to numerical instabilities which may occur.
More specifically, when 1) $n \leq 140$ and $q \leq 1 / n$, or when 2) $n \leq 140$ and $q \geq 1-1 / n$, Simard and L'Ecuyer (2011) use the Ruben and Gambino (1982) formula to calculate the distribution of $D_{n}$, returning results with at least 13 decimal digits of precision. As can be seen from Table 8 , in these regions our method gives results that are of similar accuracy as those from the pkolmim or the C program of Simard and L'Ecuyer (2011).

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :---: | :---: | :---: |
| 20 | $2.320196159531 \mathrm{E}-08$ | $2.320196159531 \mathrm{E}-08$ | $2.320196159531 \mathrm{E}-08$ | $9.9262 \mathrm{E}-23$ |
| 40 | $6.749093037884 \mathrm{E}-17$ | $6.749093037884 \mathrm{E}-17$ | $6.749093037884 \mathrm{E}-17$ | $1.7010 \mathrm{E}-30$ |
| 60 | $1.702549809333 \mathrm{E}-25$ | $1.702549809333 \mathrm{E}-25$ | $1.702549809333 \mathrm{E}-25$ | $3.0076 \mathrm{E}-39$ |
| 80 | $4.050687717856 \mathrm{E}-34$ | $4.050687717855 \mathrm{E}-34$ | $4.050687717855 \mathrm{E}-34$ | $3.2928 \mathrm{E}-47$ |
| 100 | $9.332621544394 \mathrm{E}-43$ | $9.332621544394 \mathrm{E}-43$ | $9.332621544394 \mathrm{E}-43$ | $3.4092 \mathrm{E}-56$ |
| 120 | $2.106901932614 \mathrm{E}-51$ | $2.106901932614 \mathrm{E}-51$ | $2.106901932614 \mathrm{E}-51$ | $2.5994 \mathrm{E}-64$ |
| 140 | $4.690131222300 \mathrm{E}-60$ | $4.69013122299 \mathrm{E}-60$ | $4.690131222299 \mathrm{E}-60$ | $1.0004 \mathrm{E}-72$ |

Table 8: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $q=1 / n$.
When 3) $n \leq 140$ and $1 / n<n q^{2}<0.754693$, Simard and L'Ecuyer (2011) use the Durbin matrix algorithm to calculate the distribution of $D_{n}$, returning results with at least 13 decimal digits of precision. As can be seen from Table 9, in this region our method gives results of at least the same accuracy.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: | :---: |
| 20 | 0.6089841201379 | 0.6089841201379 | 0.6089841201379 | $2.9936 \mathrm{E}-15$ |
| 40 | 0.5951497241008 | 0.5951497241008 | 0.5951497241008 | $1.9984 \mathrm{E}-15$ |
| 60 | 0.5888010590107 | 0.5888010590107 | 0.5888010590107 | $1.9984 \mathrm{E}-15$ |
| 80 | 0.5849488429478 | 0.5849488429478 | 0.5849488429478 | $4.7962 \mathrm{E}-14$ |
| 100 | 0.5822897960080 | 0.5822897960080 | 0.5822897960080 | $2.2093 \mathrm{E}-14$ |
| 120 | 0.5803108927579 | 0.5803108927579 | 0.5803108927579 | $7.2053 \mathrm{E}-14$ |
| 140 | 0.5787632928760 | 0.5787632928760 | 0.5787632928760 | $1.0991 \mathrm{E}-14$ |

Table 9: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{2}=0.75$.

When 4) $n \leq 140$ and $0.754693 \leq n q^{2}<4$, Simard and L'Ecuyer (2011) use the Pomeranz (1974) method to calculate the distribution of $D_{n}$, returning results with at least 13 decimal digits of precision. In this region, again our method gives results of at least the same accuracy as shown in Tables 10 and 11 for $n q^{2}=0.76$ and $n q^{2}=3.9$, respectively.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: | :---: |
| 20 | 0.6169412955836 | 0.6169412955835 | 0.6169412955835 | $2.9976 \mathrm{E}-15$ |
| 40 | 0.6032370735674 | 0.6032370735674 | 0.6032370735674 | $7.9936 \mathrm{E}-15$ |
| 60 | 0.5969494784897 | 0.5969494784898 | 0.5969494784897 | $9.9920 \mathrm{E}-16$ |
| 80 | 0.5931349807275 | 0.5931349807274 | 0.5931349807274 | $4.2966 \mathrm{E}-14$ |
| 100 | 0.5905022875562 | 0.5905022875562 | 0.5905022875562 | $3.0087 \mathrm{E}-14$ |
| 120 | 0.5885431553286 | 0.5885431553286 | 0.5885431553285 | $6.0063 \mathrm{E}-14$ |
| 140 | 0.5870111081551 | 0.5870111081552 | 0.5870111081551 | $1.3989 \mathrm{E}-14$ |

Table 10: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{2}=0.76$.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: | :---: |
| 20 | 0.9995468293485 | 0.9995468293485 | 0.9995468293485 | $4.9960 \mathrm{E}-15$ |
| 40 | 0.9994205337332 | 0.9994205337332 | 0.9994205337332 | $1.7097 \mathrm{E}-14$ |
| 60 | 0.9993680770022 | 0.9993680770022 | 0.9993680770022 | $1.2990 \mathrm{E}-14$ |
| 80 | 0.9993382289964 | 0.9993382289964 | 0.9993382289964 | $7.4940 \mathrm{E}-14$ |
| 100 | 0.9993185558110 | 0.9993185558110 | 0.9993185558110 | $3.9968 \mathrm{E}-14$ |
| 120 | 0.9993044245859 | 0.9993044245858 | 0.9993044245857 | $1.1902 \mathrm{E}-13$ |
| 140 | 0.9992936831012 | 0.9992936831013 | 0.9992936831012 | $1.9096 \mathrm{E}-14$ |

Table 11: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{2}=3.9$.
When 5) $n \leq 140$ and $4 \leq n q^{2}<18$, Simard and L'Ecuyer (2011) first use the Miller (1956) approximation to estimate $\mathrm{P}\left(D_{n} \geq q\right)$, and then calculate the distribution of $D_{n}$ by $\mathrm{P}\left(D_{n} \leq\right.$ $q)=1-\mathrm{P}\left(D_{n} \geq q\right)$. The authors claim that the approximated values of $\mathrm{P}\left(D_{n} \leq q\right)$ have 14 decimal digits of precision. As illustrated in Tables 12 and 13 for $n q^{2}=4.1$ and $n q^{2}=12$, our method gives results of at least the same accuracy when $n \leq 140$ and $4 \leq n q^{2} \leq 12$. For $n \leq 140$ and $12<n q^{2}<18$, since our implementation uses floating numbers in $\mathrm{C}++$, numerical instabilities may occur.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: |
| 20 | 0.99970981546296 | 0.99970981546295 | 0.99970981546295 | $5.3291 \mathrm{E}-15$ |
| 40 | 0.99962025405236 | 0.99962025405235 | 0.99962025405235 | $1.6209 \mathrm{E}-14$ |
| 60 | 0.99958292108831 | 0.99958292108830 | 0.99958292108830 | $1.6764 \mathrm{E}-14$ |
| 80 | 0.99956168530875 | 0.99956168530868 | 0.99956168530868 | $7.5717 \mathrm{E}-14$ |
| 100 | 0.99954770168480 | 0.99954770168484 | 0.99954770168484 | $4.3188 \mathrm{E}-14$ |
| 120 | 0.99953766763972 | 0.99953766763961 | 0.99953766763961 | $1.1346 \mathrm{E}-13$ |
| 140 | 0.99953004813548 | 0.99953004813546 | 0.99953004813546 | $1.8430 \mathrm{E}-14$ |

Table 12: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{2}=4.1$.

When 6) $n \leq 140$ and $n q^{2} \geq 18, \mathrm{P}\left(D_{n} \geq q\right)<5 \times 10^{-16}$. Equivalently, $\mathrm{P}\left(D_{n} \leq q\right)=$

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: |
| 20 | 0.99999999999963 | 0.99999999999962 | 0.99999999999962 | $7.5495 \mathrm{E}-15$ |
| 40 | 0.99999999999135 | 0.99999999999134 | 0.99999999999134 | $1.5210 \mathrm{E}-14$ |
| 60 | 0.99999999998168 | 0.99999999998167 | 0.99999999998167 | $1.3656 \mathrm{E}-14$ |
| 80 | 0.99999999997415 | 0.99999999997407 | 0.99999999997407 | $7.6827 \mathrm{E}-14$ |
| 100 | 0.99999999996823 | 0.99999999996827 | 0.99999999996827 | $3.8192 \mathrm{E}-14$ |
| 120 | 0.99999999996388 | 0.99999999996376 | 0.99999999996376 | $1.1702 \mathrm{E}-13$ |
| 140 | 0.99999999996020 | 0.99999999996017 | 0.99999999996017 | $2.3981 \mathrm{E}-14$ |

Table 13: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{2}=12$.
$1-\mathrm{P}\left(D_{n} \geq q\right)>1-5 \times 10^{-16}$. Hence, returning $\mathrm{P}\left(D_{n} \leq q\right)=1$ will give results with 15 decimal digits of precision.
When 7) $140<n \leq 10^{5}$ and $n q^{3 / 2}<1.4$, Simard and L'Ecuyer (2011) use the Durbin matrix algorithm to obtain the exact distribution of $D_{n}$, returning probabilities with at least 13 decimal digits of precision. As illustrated in Table 14, our method returns values of at least the same accuracy.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :---: | :---: | :---: |
| 140 | $6.378698330645 \mathrm{E}-02$ | $6.378698330644 \mathrm{E}-02$ | $6.378698330644 \mathrm{E}-02$ | $9,9920 \mathrm{E}-16$ |
| 200 | $3.847020660831 \mathrm{E}-02$ | $3.847020660831 \mathrm{E}-02$ | $3.847020660831 \mathrm{E}-02$ | $4.9960 \mathrm{E}-16$ |
| 500 | $7.365490405433 \mathrm{E}-03$ | $7.365490405433 \mathrm{E}-03$ | $7.365490405433 \mathrm{E}-03$ | $3.9899 \mathrm{E}-17$ |
| 1000 | $1.383862966203 \mathrm{E}-03$ | $1.383862966202 \mathrm{E}-03$ | $1.383862966202 \mathrm{E}-03$ | $3.7015 \mathrm{E}-16$ |
| 2000 | $1.629201120187 \mathrm{E}-04$ | $1.629201120188 \mathrm{E}-04$ | $1.629201120188 \mathrm{E}-04$ | $1.5501 \mathrm{E}-16$ |
| 5000 | $3.811342214264 \mathrm{E}-06$ | $3.811342214276 \mathrm{E}-06$ | $3.811342214276 \mathrm{E}-06$ | $1.1910 \mathrm{E}-17$ |
| 10000 | $8.999089573402 \mathrm{E}-08$ | $8.999089573401 \mathrm{E}-08$ | $8.999089573401 \mathrm{E}-08$ | $1.2308 \mathrm{E}-20$ |
| 100000 | $5.388085736386 \mathrm{E}-17$ | $5.388085736343 \mathrm{E}-17$ | $5.388085736345 \mathrm{E}-17$ | $4.0739 \mathrm{E}-28$ |

Table 14: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{3 / 2}=1.3$.

In region 8), when $140<n \leq 10^{5}, n q^{3 / 2} \geq 1.4$, and $n q^{2} \leq 18$, Simard and L'Ecuyer (2011) apply the Pelz and Good (1976) approximation that gives five decimal digits of precision for values of $\mathrm{P}\left(D_{n} \leq q\right)$. In contrast, when $140<n \leq 10^{5}, n q^{3 / 2} \geq 1.4$, and $n q^{2} \leq 10$, our approach gives results with at least 11 decimal digits of precision even though it is using floating numbers in calculation. The results when $n q^{3 / 2}=1.4$ and when $n q^{2}=10$ are shown in Tables 15 and 16 , respectively. However, in region 8 ), when $140<n \leq 10^{5}, n q^{3 / 2} \geq 1.4$, and $n q^{2}>10$, our approach may be unsuitable due to numerical instabilities. In particular, it will return results with at least 11 decimal digits of precision, but the resulting values of $\mathrm{P}\left(D_{n} \leq q\right)$ may not be decreasing in $n$, due to the errors in calculations with floating numbers. When $140<n \leq 10^{5}$ and $n q^{2} \geq 18$, returning $\mathrm{P}\left(D_{n} \leq q\right)=1$ will give results with 15 decimal digits of precision.
Finally, in region 9), Simard and L'Ecuyer (2011) apply the Pelz and Good (1976) approximation to obtain values of $\mathrm{P}\left(D_{n} \leq q\right)$ when $n q^{2}<18$, and set $\mathrm{P}\left(D_{n} \leq q\right)=1$ when $n q^{2} \geq 18$. As illustrated in Table 17 for $n=100001$, our approach tends to be more accurate when $\mathrm{P}\left(D_{n} \leq q\right)$ is very small. However, Pelz and Good (1976) approximation may provide higher accuracy when $\mathrm{P}\left(D_{n} \leq q\right)$ tends to one.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: | :---: |
| 140 | $9.0262329475006 \mathrm{E}-02$ | $9.025921823 \mathrm{E}-02$ | $9.0262329475004 \mathrm{E}-02$ | $1.9013 \mathrm{E}-15$ |
| 500 | $1.3024254002106 \mathrm{E}-02$ | $1.302426466 \mathrm{E}-02$ | $1.3024254002106 \mathrm{E}-02$ | $4.0072 \mathrm{E}-16$ |
| 1000 | $2.8949372516988 \mathrm{E}-03$ | $2.89496818 \mathrm{E}-03$ | $2.8949372516981 \mathrm{E}-03$ | $6.7004 \mathrm{E}-16$ |
| 5000 | $1.4235508314598 \mathrm{E}-05$ | $1.42356151 \mathrm{E}-05$ | $1.4235508314645 \mathrm{E}-05$ | $4.7100 \mathrm{E}-17$ |
| 10000 | $4.8334541076751 \mathrm{E}-07$ | $4.83345438 \mathrm{E}-08$ | $4.8334541076707 \mathrm{E}-07$ | $4.3506 \mathrm{E}-19$ |
| 50000 | $3.7148003980197 \mathrm{E}-12$ | $3.71479094 \mathrm{E}-12$ | $3.7147909440549 \mathrm{E}-12$ | $9.4540 \mathrm{E}-18$ |
| 100000 | $2.2123605255202 \mathrm{E}-15$ | $2.21229903 \mathrm{E}-15$ | $2.2123605254766 \mathrm{E}-15$ | $4.3560 \mathrm{E}-26$ |

Table 15: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{3 / 2}=1.4$.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: | :---: |
| 141 | 0.99999999743970 | 0.99999999743965 | 0.99999999743964 | $5.6066 \mathrm{E}-14$ |
| 500 | 0.99999999654196 | 0.99999999654197 | 0.99999999654196 | $9.9920 \mathrm{E}-16$ |
| 1000 | 0.99999999629650 | 0.99999999629831 | 0.99999999629630 | $1.9806 \mathrm{E}-13$ |
| 5000 | 0.99999999602730 | 0.99999999603085 | 0.99999999603074 | $3.4379 \mathrm{E}-12$ |
| 10000 | 0.99999999597940 | 0.99999999597986 | 0.99999999597981 | $4.1001 \mathrm{E}-13$ |
| 50000 | 0.9999999592690 | 0.99999999591965 | 0.99999999591967 | $7.2330 \mathrm{E}-12$ |
| 100000 | 0.99999999592133 | 0.99999999590672 | 0.99999999590684 | $1.4486 \mathrm{E}-11$ |

Table 16: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n q^{2}=10$.

| $q$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| :---: | :---: | :--- | :---: | :---: |
| $\frac{1}{10 \sqrt{n}}$ | $2.350089150939 \mathrm{E}-52$ | $2.269812367 \mathrm{E}-52$ | $2.350089151281 \mathrm{E}-52$ | $3.4177 \mathrm{E}-62$ |
| $\frac{1}{8 \sqrt{n}}$ | $1.969026572915 \mathrm{E}-33$ | $1.962478061 \mathrm{E}-33$ | $1.969026573193 \mathrm{E}-33$ | $2.7816 \mathrm{E}-43$ |
| $\frac{1}{6 \sqrt{n}}$ | $1.018454527586 \mathrm{E}-18$ | $1.018350563 \mathrm{E}-18$ | $1.018454527742 \mathrm{E}-18$ | $1.5595 \mathrm{E}-28$ |
| $\frac{1}{4 \sqrt{n}}$ | $2.907074248741 \mathrm{E}-08$ | $2.9070737934 \mathrm{E}-08$ | $2.907074249157 \mathrm{E}-08$ | $4.1588 \mathrm{E}-18$ |
| $\frac{1}{2 \sqrt{n}}$ | $3.639199759592 \mathrm{E}-02$ | $3.639199759592 \mathrm{E}-02$ | $3.639199760172 \mathrm{E}-02$ | $5.7979 \mathrm{E}-12$ |
| $\frac{1}{\sqrt{n}}$ | $7.305646850557 \mathrm{E}-01$ | $7.305646847185 \mathrm{E}-01$ | $7.305646847159 \mathrm{E}-01$ | $3.3980 \mathrm{E}-10$ |
| $\frac{2}{\sqrt{n}}$ | $9.993319331457 \mathrm{E}-01$ | $9.993319333086 \mathrm{E}-01$ | $9.993319333086 \mathrm{E}-01$ | $1.6290 \mathrm{E}-10$ |

Table 17: Values of $\mathrm{P}\left(D_{n} \leq q\right)$ for $n=100001$.

To conclude, apart from the regions where $n \leq 140$ and $12<n q^{2}<18$; or $140<n \leq 10^{5}$, $n q^{3 / 2} \geq 1.4$, and $10<n q^{2}<18$; or $n q^{2} \geq 18$, the Exact-KS-FFT method returns values of $\mathrm{P}\left(D_{n} \leq q\right)$ that are at least as accurate as those obtained by Simard and L'Ecuyer (2011). This is shown in Figure 4. Moreover, for $n>10^{5}$, the proposed method may be accurate when $\mathrm{P}\left(D_{n} \leq q\right)$ is very small.


Figure 4: Approximate regions where the Exact-KS-FFT method returns $\mathrm{P}\left(D_{n} \leq q\right)$ efficiently and accurately.

## C. Computing the complementary cdf when $F(x)$ is continuous: numerical analysis and comparisons

It is well known that

$$
D_{n}=\sup _{x}\left|F_{n}(x)-F(x)\right| \longrightarrow 0 \quad \text { a.s. },
$$

as $n \rightarrow \infty$. Hence, when $n$ is very large, $\mathrm{P}\left(D_{n} \leq q\right)$ is close to one. Also, it can be seen that $D_{n} \in[0,1]$, so $\mathrm{P}\left(D_{n} \leq q\right)$ is close to one when $q$ is close to one. In these cases, cancellation errors may occur when trying to numerically compute the $p$ value

$$
\begin{equation*}
\mathrm{P}\left(D_{n} \geq q\right)=1-\mathrm{P}\left(D_{n} \leq q\right) . \tag{29}
\end{equation*}
$$

Similarly to previous section, we compute the values of $\mathrm{P}\left(D_{n} \geq q\right)$ for different $n$ and $q$ using the Exact-KS-FFT method and compare the results to those obtained with the R program of Carvalho (2015), and the C program due to Simard and L'Ecuyer (2011).
In order to compute $\mathrm{P}\left(D_{n} \geq q\right)$, when $F(x)$ is continuous using the R package KSgeneral, one needs to input cont_ks_c_cdf( $\mathrm{q}, \mathrm{n}$ ). For instance, in order to compute the value for $\mathrm{P}\left(D_{n} \geq q\right)$, for $n=141, n q^{2}=2.1$, one should run the following R code and obtain the corresponding result as shown in Table 19 for $n=141$ in the column Exact-KS-FFT.
$R>$ cont_ks_c_cdf(sqrt(2.1/141), 141)
[1] 0.02743689

Simard and L'Ecuyer (2011) consider the following regions: 1) $n \leq 140$ and $n q^{2}<4$; 2) $n \leq 140$ and $n q^{2} \geq 4$; 3) $n>140$ and $n q^{2}<2.2$; and 4) $n>140$ and $n q^{2} \geq 2.2$ where they use different methods to compute the complementary cdf of $D_{n}$ (cf., Simard and L'Ecuyer 2011, Section 5).
Following the segmentation of regions, we have computed the complementary cdf of $D_{n}$ with the proposed FFT-based method. Consequently, we can report that for region 1), our approach gives results that are of at least the same accuracy as those obtained from the R or C program. In region 2$), \mathrm{P}\left(D_{n} \leq q\right)$ is close to one and our method may be unsuitable due to cancellation errors which may occur when calculating the complementary cdf via (29). A comparison for $n q^{2}=4$ is shown in Table 18 .

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: | :---: |
| 20 | $3.627396978 \mathrm{E}-04$ | $3.627396978 \mathrm{E}-04$ | $3.627396978 \mathrm{E}-04$ | $5.0590 \mathrm{E}-15$ |
| 40 | $4.691487961 \mathrm{E}-04$ | $4.691487961 \mathrm{E}-04$ | $4.691487961 \mathrm{E}-04$ | $1.5461 \mathrm{E}-14$ |
| 60 | $5.134182982 \mathrm{E}-04$ | $5.134182982 \mathrm{E}-04$ | $5.134182982 \mathrm{E}-04$ | $1.3937 \mathrm{E}-14$ |
| 80 | $5.386021475 \mathrm{E}-04$ | $5.386021476 \mathrm{E}-04$ | $5.386021476 \mathrm{E}-04$ | $7.4480 \mathrm{E}-14$ |
| 100 | $5.551927328 \mathrm{E}-04$ | $5.551927328 \mathrm{E}-04$ | $5.551927328 \mathrm{E}-04$ | $3.9403 \mathrm{E}-14$ |
| 120 | $5.671032850 \mathrm{E}-04$ | $5.671032851 \mathrm{E}-04$ | $5.671032851 \mathrm{E}-04$ | $1.0974 \mathrm{E}-13$ |
| 140 | $5.761521040 \mathrm{E}-04$ | $5.761521040 \mathrm{E}-04$ | $5.761521040 \mathrm{E}-04$ | $1.0433 \mathrm{E}-14$ |

Table 18: Values of $\mathrm{P}\left(D_{n} \geq q\right)$ for $n q^{2}=4$.
In region 3), when $140<n \leq 10^{5}$ and $n q^{2}<2.2$, Simard and L'Ecuyer (2011) use the Pelz and Good (1976) approximation and apply (29) to calculate the complementary cdf, returning results with at least five decimal digits of precision. Our approach also applies (29), but returns results with at least nine decimal digits of precision. A comparison for $n q^{2}=2.1$ is given in Table 19.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :--- | :--- | :---: | :---: |
| 141 | 0.02743688914 | 0.02743688914 | 0.02743688914 | $5.0990 \mathrm{E}-13$ |
| 500 | 0.02866250067 | 0.02866250067 | 0.02866250073 | $5.9554 \mathrm{E}-11$ |
| 1000 | 0.02905830855 | 0.02905830855 | 0.02905830828 | $2.6492 \mathrm{E}-10$ |
| 5000 | 0.02957796836 | 0.02957796836 | 0.02957796797 | $3.9119 \mathrm{E}-10$ |
| 10000 | 0.02969964497 | 0.02969964497 | 0.02969964418 | $7.9672 \mathrm{E}-10$ |
| 50000 | 0.02986114255 | 0.02986114255 | 0.02986114263 | $7.2066 \mathrm{E}-11$ |
| 100000 | 0.02989926133 | 0.02989926162 | 0.02989926162 | $2.8962 \mathrm{E}-10$ |

Table 19: Values of $\mathrm{P}\left(D_{n} \geq q\right)$ for $n q^{2}=2.1$.
In region 4), when $140<n \leq 10^{5}$ and $n q^{2} \geq 2.2$, Simard and L'Ecuyer (2011) use the Miller (1956) approximation and obtain complementary cdf with at least six decimal digits of precision. In this region, the proposed FFT-based method may give more accurate results when $140<n \leq 10^{5}$ and $2.2 \leq n q^{2} \leq 7$. For example, for $n q^{2}=2.2$ and $n q^{2}=7$, Tables 20 and 21 show that the Exact-KS-FFT method returns complementary cdf with at least 10 decimal digits of precision. When $140<n \leq 10^{5}$ and $n q^{2}>7$, our method may be unsuitable due to cancellation errors as previously discussed.
Finally, when $n>10^{5}$ and $n q^{2}<370$, Simard and L'Ecuyer (2011) use the Miller (1956) approximation and obtain complementary cdf with a few correct decimal digits. These authors

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :--- | :--- | :---: | :---: |
| 141 | 0.02239633302 | 0.0223963592 | 0.02239633302 | $5.2000 \mathrm{E}-14$ |
| 500 | 0.02343606481 | 0.0234361007 | 0.02343606481 | $2.6201 \mathrm{E}-14$ |
| 1000 | 0.02377033994 | 0.0237703789 | 0.02377033994 | $2.0260 \mathrm{E}-13$ |
| 10000 | 0.02431016270 | 0.0243102062 | 0.02431016270 | $1.3636 \mathrm{E}-12$ |
| 100000 | 0.02447768608 | 0.0244777310 | 0.02447768610 | $1.8812 \mathrm{E}-11$ |

Table 20: Values of $\mathrm{P}\left(D_{n} \geq q\right)$ for $n q^{2}=2.2$.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| ---: | :---: | :--- | :---: | :---: |
| 141 | $1.2484862 \mathrm{E}-06$ | $1.2484863 \mathrm{E}-06$ | $1.2484863 \mathrm{E}-06$ | $5.7535 \mathrm{E}-14$ |
| 500 | $1.4796907 \mathrm{E}-06$ | $1.4796906 \mathrm{E}-06$ | $1.4796907 \mathrm{E}-06$ | $2.1112 \mathrm{E}-14$ |
| 1000 | $1.5434598 \mathrm{E}-06$ | $1.5434599 \mathrm{E}-06$ | $1.5434600 \mathrm{E}-06$ | $1.9722 \mathrm{E}-13$ |
| 10000 | $1.6309268 \mathrm{E}-06$ | $1.6309265 \mathrm{E}-06$ | $1.6309266 \mathrm{E}-06$ | $1.9895 \mathrm{E}-13$ |
| 100000 | $1.6534902 \mathrm{E}-06$ | $1.6534983 \mathrm{E}-06$ | $1.6534982 \mathrm{E}-06$ | $7.9321 \mathrm{E}-12$ |

Table 21: Values of $\mathrm{P}\left(D_{n} \geq q\right)$ for $n q^{2}=7$.
have shown that complementary cdf can be set to be zero when $n q^{2} \geq 370$. Recall that in Table 17, we have shown that the Exact-KS-FFT method tends to be more accurate when $\mathrm{P}\left(D_{n} \leq q\right)$ is very small, or when $q$ is small. In this case, we can apply (29) to calculate the complementary cdf, without incurring large cancellation errors. More specifically, when $n>10^{5}$ and $n q^{2} \leq 3$, the Exact-KS-FFT method returns complementary cdf with at least seven decimal digits of precision as demonstrated in Table 22. The accuracy of course deteriorates when $n>10^{5}$ and $3<n q^{2}<370$.

| $n$ | Exact-KS-FFT | Simard \& L'Ecuyer | Carvalho | Abs. err. |
| :---: | :---: | :--- | :---: | :---: |
| 100001 | $4.939303411 \mathrm{E}-03$ | $4.939303336 \mathrm{E}-03$ | $4.939303263053 \mathrm{E}-03$ | $1.4795 \mathrm{E}-10$ |
| 200000 | $4.944654927 \mathrm{E}-03$ | $4.944654662 \mathrm{E}-03$ | $4.944654584319 \mathrm{E}-03$ | $3.4268 \mathrm{E}-10$ |
| 300000 | $4.947020044 \mathrm{E}-03$ | $4.947020013 \mathrm{E}-03$ | $4.947019946709 \mathrm{E}-03$ | $9.7291 \mathrm{E}-11$ |

Table 22: Values of $\mathrm{P}\left(D_{n} \geq q\right)$ for $n q^{2}=3$.
To summarize, apart from the regions where $n \leq 140$ and $n q^{2} \geq 4$; or $n \leq 140$ and $q \geq 1-1 / n$; or $140<n \leq 10^{5}$ and $n q^{2}>7$, the Exact-KS-FFT method returns values of the probability $\mathrm{P}\left(D_{n} \geq q\right)$ that are at least as accurate as those obtained by Simard and L'Ecuyer (2011). This is shown in Figure 5. Moreover, when $n>10^{5}$ and $n q^{2} \leq 3$, the proposed approach may be more accurate than Simard and L'Ecuyer (2011) method.

## D. Speed comparison

Tables 23,24 and 25 report the CPU times to compute $\mathrm{P}\left(D_{n} \geq q\right) 100$ times, for selected values of $n$ and $\lambda$. Note that Carvalho (2015) procedure cannot be used with the chosen values of $q$ and $n=100000$ as it is prohibitively slow. As expected, Simard and L'Ecuyer (2011) C program which combines the most efficient methods for computing the distribution of $D_{n}$ for $F(x)$ continuous, is the fastest among the three procedures. However, the Exact-KS-FFT


Figure 5: Approximate regions where the Exact-KS-FFT method returns $\mathrm{P}\left(D_{n} \geq q\right)$ efficiently and accurately
method proves to be a viable alternative especially given its generality and applicability to the case of discontinuous $F(x)$.

| $n \backslash \lambda$ | 0.25 | 0.5 | 1 | 2 | 3 | 4 |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 10 | 0.00034 | 0.00059 | 0.00065 | 0.00069 | 0.00087 | 0.00014 |
| 100 | 0.00524 | 0.01318 | 0.01835 | 0.03242 | 0.04765 | 0.00107 |
| 140 | 0.00615 | 0.01915 | 0.03474 | 0.06172 | 0.08618 | 0.11874 |
| 141 | 0.00673 | 0.01955 | 0.03529 | 0.06657 | 0.09285 | 0.11886 |
| 1000 | 0.15040 | 0.00013 | 0.00014 | 0.00019 | 0.00894 | 0.00894 |
| 10000 | 0.00013 | 0.00014 | 0.00012 | 0.00015 | 0.08124 | 0.08080 |
| 100000 | 0.00014 | 0.00015 | 0.00014 | 0.00019 | 0.78912 | 0.75099 |

Table 23: CPU time (seconds) to compute $\mathrm{P}\left(D_{n} \geq q\right) 100$ times with the Simard and L'Ecuyer (2011) C program.

| $n \backslash \lambda$ | 0.25 | 0.5 | 1 | 2 | 3 | 4 |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 10 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 100 | 0.0150 | 0.0150 | 0.0150 | 0.0380 | 0.0380 | 0.0550 |
| 140 | 0.0150 | 0.0150 | 0.0310 | 0.0620 | 0.0780 | 0.1090 |
| 141 | 0.0150 | 0.0150 | 0.0310 | 0.0620 | 0.0780 | 0.1090 |
| 1000 | 0.1400 | 0.2960 | 0.6550 | 1.1700 | 1.9340 | 2.2990 |
| 10000 | 5.6310 | 8.5320 | 19.500 | 45.100 | 52.890 | 94.700 |
| 100000 | 182.29 | 333.31 | 672.16 | 1466.6 | 2503.3 | 3211.7 |

Table 24: CPU time (seconds) to compute $\mathrm{P}\left(D_{n} \geq q\right) 100$ times with the Exact-KS-FFT method.

| $n \backslash \lambda$ | 0.25 | 0.5 | 1 | 2 | 3 | 4 |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 10 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| 100 | 0.003 | 0.004 | 0.006 | 0.009 | 0.013 | 0.017 |
| 140 | 0.004 | 0.006 | 0.009 | 0.014 | 0.020 | 0.023 |
| 141 | 0.004 | 0.006 | 0.009 | 0.014 | 0.020 | 0.024 |
| 1000 | 0.086 | 0.155 | 0.268 | 0.499 | 0.747 | 1.066 |
| 10000 | 6.250 | 13.16 | 40.22 | 97.18 | 145.5 | 188.4 |
| 100000 | na | na | na | na | na | na |

Table 25: CPU time (seconds) to compute $\mathrm{P}\left(D_{n} \geq q\right) 100$ times with the Carvalho (2015) R program.

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[^0]:    ${ }^{1}$ An expression similar to (5) for the case of $\mathrm{P}\left(D_{n}>q\right)$ has been obtained by Gleser (1985) (cf., Theorem 2 therein).

[^1]:    ${ }^{2}$ Both Khmaladze and Shinjikashvili (2001) and Moscovich and Nadler (2017) assume $F(x)$ is continuous and consider strict inequalities in (8) i.e., they do not allow the process to touch the boundaries.

