SSJ User's Guide

Package `gof`

Goodness-of-fit test Statistics

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This package provides facilities for performing and reporting different types of univariate goodness-of-fit statistical tests.

Contents

Overview

This package contains tools for performing univariate *goodness-of-fit* (GOF) statistical tests. Static methods for computing (or approximating) the distribution function $F(x)$ of certain GOF test statistics, as well as their complementary distribution function $\bar{F}(x) = 1 - F(x)$, are implemented in classes `FDist` and `FBar`. Tools for computing the GOF test statistics and the corresponding p-values, and for formating the results, are provided in classes `GofStat` and `GofFormat`.

We are concerned here with GOF test statistics for testing the hypothesis $\mathcal{H}_0$ that a sample of N observations $X_1, \dots, X_N$ comes from a given univariate probability distribution F. We consider tests such as those of Kolmogorov-Smirnov, Anderson-Darling, Crámer-von Mises, etc. These test statistics generally measure, in different ways, the distance between a *continuous* distribution function F and the *empirical distribution function* (EDF) $\hat{F}_N$ of $X_1, \dots, X_N$. They are also called EDF test statistics. The observations X_i are usually transformed into $U_i = F(X_i)$, which satisfy $0 \le U_i \le 1$ and which follow the $U(0, 1)$ distribution under $\mathcal{H}_0$. (This is called the *probability integral transformation*.) Methods for applying this transformation, as well as other types of transformations, to the observations X_i or U_i are provided in `GofStat`.

Then the GOF tests are applied to the U_i sorted by increasing order. The corresponding p-values are easily computed by calling the appropriate static methods in `FDist`. If a GOF test statistic Y has a continuous distribution under $\mathcal{H}_0$ and takes the value y, its (right) p-value is defined as $p = P[Y \ge y \mid \mathcal{H}_0]$. The test usually rejects $\mathcal{H}_0$ if p is deemed too close to 0 (for a one-sided test) or too close to 0 or 1 (for a two-sided test).

In the case where Y has a *discrete distribution* under $\mathcal{H}_0$, we distinguish the *right p-value* $p_R = P[Y \ge y \mid \mathcal{H}_0]$ and the *left p-value* $p_L = P[Y \le y \mid \mathcal{H}_0]$. We then define the p-value for a two-sided test as

$$p = \begin{cases} p_R, & \text{if } p_R < p_L \\ 1 - p_L, & \text{if } p_R \ge p_L \text{ and } p_L < 0.5 \\ 0.5 & \text{otherwise.} \end{cases} \tag{1}$$

Why such a definition? Consider for example a Poisson random variable Y with mean 1 under $\mathcal{H}_0$. If Y takes the value 0, the right p-value is $p_R = P[Y \ge 0 \mid \mathcal{H}_0] = 1$. In the uniform case, this would obviously lead to rejecting $\mathcal{H}_0$ on the basis that the p-value is too close to 1. However, $P[Y = 0 \mid \mathcal{H}_0] = 1/e \approx 0.368$, so it does not really make sense to reject $\mathcal{H}_0$ in this case. In fact, the left p-value here is $p_L = 0.368$, and the p-value computed with the above definition is $p = 1 - p_L \approx 0.632$. Note that if p_L is very small, in this definition, p becomes close to 1. If the left p-value was defined as $p_L = 1 - p_R = P[Y < y \mid \mathcal{H}_0]$, this would also lead to problems. In the example, one would have $p_L = 0$ in that case.

A very common type of test in the discrete case is the *chi-square* test, which applies when the possible outcomes are partitioned into a finite number of categories. Suppose there are k categories and that each observation belongs to category i with probability p_i, for $0 \le i < k$.

If there are n independent observations, the expected number of observations in category i is $e_i = np_i$, and the chi-square test statistic is defined as

$$X^2 = \sum_{i=0}^{k-1} \frac{(o_i - e_i)^2}{e_i} \tag{2}$$

where o_i is the actual number of observations in category i. Assuming that all e_i's are large enough (a popular rule of thumb asks for $e_i \geq 5$ for each i), X^2 follows approximately the chi-square distribution with $k - 1$ degrees of freedom [15]. The class `GofStat.OutcomeCategoriesChi2`, a nested class defined inside the `GofStat` class, provides tools to automatically regroup categories in the cases where some e_i's are too small.

The class `GofFormat` contains methods used to format results of GOF test statistics, or to apply several such tests simultaneously to a given data set and format the results to produce a report that also contains the p-values of all these tests. A C version of this class is actually used extensively in the package TestU01, which applies statistical tests to random number generators [12]. The class also provides tools to plot an empirical or theoretical distribution function, by creating a data file that contains a graphic plot in a format compatible with a given software.

FDist

WARNING: Most methods in this class are **deprecated**. The method `cdf` of the appropriate class in package `probdist` should be used instead.

This class provides methods to compute (or approximate) the distribution functions of various types of goodness-of-fit test statistics. All the methods in this class return $F(x)$ for some probability distribution. Recall that the distribution function of a continuous random variable X with density f is

$$F(x) = P[X \le x] = \int_{-\infty}^{x} f(x)dx \tag{3}$$

while that of a discrete random variable X with mass function f over the set of integers is

$$F(x) = P[X \le x] = \sum_{s=-\infty}^{x} f(s). \tag{4}$$

Most distributions are implemented only in standardized form here, i.e., with the location parameter set to 0 and the scale parameter set to 1. To shift the distribution by x_0 and rescale by c, it suffices to replace x by $(x - x_0)/c$ in the argument when calling the function.

```
package umontreal.iro.lecuyer.gof;
```

```
public class FDist
```

```
@Deprecated
public static double kolmogorovSmirnovPlus (int N, double x)
```

Use `KolmogorovSmirnovPlusDist.cdf(N, x)` **instead.**

Returns $p(x) = P[D_N^+ \le x]$, where

$$D_N^+ = \sup_{-\infty < s < \infty} [\hat{F}_N(s) - F(s)]^+ \tag{5}$$

is the Kolmogorov-Smirnov+ statistic for a sample of size N whose empirical distribution function is $\hat{F}_N$, under the hypothesis that the observations follow a continuous distribution function F. (Recall that x^+ represents $\max(0, x)$, the positive part of x.) The statistic

$$D_N^- = \sup_{-\infty < s < \infty} [F(s) - \hat{F}_N(s)]^+ \tag{6}$$

has the same distribution as D_N^+. Methods for computing these statistics are available in class `GofStat`. The distribution function of D_N^+ can be approximated via the following expressions:

$$
\begin{aligned}
P[D_N^+ \le x] &= 1 - x \sum_{i=0}^{\lfloor N(1-x)\rfloor} \binom{N}{i} \left(\frac{i}{N} + x\right)^{i-1} \left(1 - \frac{i}{N} - x\right)^{N-i} &(7)\\
&= x \sum_{j=0}^{\lfloor Nx\rfloor} \binom{N}{j} \left(\frac{j}{N} - x\right)^{j} \left(1 - \frac{j}{N} + x\right)^{N-j-1} &(8)\\
&\approx 1 - e^{-2Nx^2} \left[1 - \frac{2x}{3}\left(1 - x\left(1 - \frac{2Nx^2}{3}\right)\right.\right.\\
&\quad \left.\left. - \frac{2}{3N}\left(\frac{1}{5} - \frac{19Nx^2}{15} + \frac{2N^2x^4}{3}\right)\right) + O(N^{-2})\right]. &(9)
\end{aligned}
$$

Formula (7) and (8) can be found in [5], equations (2.1.12) and (2.1.16), while (9) can be found in [3]. Formula (8) contains less terms than (7) when $x < 0.5$, but becomes numerically unstable as Nx increases, because its terms alternate in sign and become large (in absolute value) compared to their sum. The approximation (9) is simpler to compute and excellent when Nx is large. Our implementation uses (8) when $Nx < 6.5$, (7) when $Nx \ge 6.5$ and $N \le 100$, and (9) when $Nx \ge 6.5$ and $N > 100$. The relative error on $p(x) = P[D_N^+ \le x]$ is always less than 10^{-5}, and the relative error on $1 - p(x)$ is less than 10^{-1} when $1 - p(x) > 10^{-10}$. The *absolute* error on $1 - p(x)$ is less than 10^{-11} when $1 - p(x) < 10^{-10}$.

```
@Deprecated
public static double kolmogorovSmirnov (int N, double x)
```

Use `KolmogorovSmirnovDistQuick.cdf(N, x)` instead. Returns $p(x) = P[D_N \le x]$, where $D_N = \max(D_N^+, D_N^-)$ is the two-sided Kolmogorov-Smirnov statistic for a sample of size N and where D_N^+ and D_N^- are defined in (5) and (6). Uses the approximation given in corollary Z of [3], page 356. This approximation improves when N increase or x goes away from 0. The error on $p(x)$ is less than 1 percent (approximately) for $N > 100$.

Warning: for $1 < N < 10$ or x in the lower tail, the approximation is bad. But the precision is at least 1 decimal digit nearly everywhere.

```
public static double kolmogorovSmirnovPlusJumpOne (int N, double a,
                                                   double x)
```

Similar to `kolmogorovSmirnovPlus` but for the case where the distribution function F has a jump of size a at a given point x_0, is zero at the left of x_0, and is continuous at the right of x_0. The Kolmogorov-Smirnov statistic is defined in that case as

$$D_N^+(a) = \sup_{a \le u \le 1} \left(\hat{F}_N(F^{-1}(u)) - u\right) = \max_{\lfloor 1 + aN \le j \le N} \left(j/N - F(V_{(j)})\right). \tag{10}$$

where $V_{(1)}, \ldots, V_{(N)}$ are the observations sorted by increasing order. The method returns an approximation of $P[D_N^+(a) \le x]$ computed via

$$P[D_N^+(a) \le x] \;=\; 1 - x \sum_{i=0}^{\lfloor N(1-a-x)\rfloor} \binom{N}{i} \left(\frac{i}{N} + x\right)^{i-1} \left(1 - \frac{i}{N} - x\right)^{N-i}. \qquad (11)$$

$$= \; x \sum_{j=0}^{\lfloor N(a+x)\rfloor} \binom{N}{j} \left(\frac{j}{N} - x\right)^{j} \left(1 - \frac{j}{N} + x\right)^{N-j-1}. \qquad (12)$$

The current implementation uses formula (12) when $N(x+a) < 6.5$ and $x + a < 0.5$, and uses (11) when $Nx \ge 6.5$ or $x + a \ge 0.5$. Restriction: $0 < a < 1$.

```
@Deprecated
public static double cramerVonMises (int N, double x)
```

Use `CramerVonMisesDist.cdf(N, x)` instead. Returns an approximation of $P[W_N^2 \le x]$, where W_N^2 is the Cramér-von Mises statistic (see [16, 17, 2, 8]) defined in (19), for a sample of independent uniforms over $(0, 1)$. The approximation is based on the distribution function of $W^2 = \lim_{N\to\infty} W_N^2$, which has the following series expansion derived by Anderson and Darling [2]:

$$P(W^2 \le x) \;=\; \frac{1}{\pi\sqrt{x}} \sum_{j=0}^{\infty} (-1)^j \binom{-1/2}{j} \sqrt{4j+1}\; \exp\left(-\frac{(4j+1)^2}{16x}\right) \mathrm{K}_{1/4}\left(\frac{(4j+1)^2}{16x}\right),$$

where K_ν is the modified Bessel function of the second kind. To correct for the deviation between $P(W_N^2 \le x)$ and $P(W^2 \le x)$, we add a correction in $1/N$, obtained empirically by simulation. For $N = 10, 20, 40$, the error is less than 0.002, 0.001, and 0.0005, respectively, while for $N \ge 100$ it is less than 0.0005. For $N \to \infty$, we estimate that the method returns at least 6 decimal digits of precision. For $N = 1$, the method computes the exact distribution: $P(W_1^2 \le x) = 2\sqrt{x - 1/12}$ for $1/12 \le x \le 1/3$.

```
@Deprecated
public static double watsonU (int N, double x)
```

Use `WatsonUDist.cdf(N, x)` instead. Returns $P[U^2 \le x]$, where U^2 is the Watson statistic defined in (22) in the limit when $N \to \infty$, for a sample of independent uniforms over $(0, 1)$. Only this limiting distribution (when $N \to \infty$) is implemented. It is given by

$$P(U^2 \le x) \;=\; 1 + 2\sum_{j=1}^{\infty} (-1)^j e^{-2j^2\pi^2 x} \qquad (13)$$

This sum converges extremely fast except for small x, where alternating successive terms give rise to numerical instability. But with the Poisson summation formula [10], the sum can be transformed to

$$P(U^2 \le x) \;=\; \sqrt{\frac{2}{\pi x}} \sum_{j=0}^{\infty} e^{-(2j+1)^2/8x} \qquad (14)$$

which can be used for small x. The current implementation uses (13) for $x > 0.15$, and (14) for $x \le 0.15$. The absolute difference between the returned value and $P[U_N^2 \le x]$ is estimated to be less than 0.01 for $N \ge 8$.

```
@Deprecated
public static double watsonG (int N, double x)
```

Use `WatsonGDist.cdf(N, x)` instead. Returns an approximation of $P[G_N \le x]$, where G_N is the Watson statistic defined in (20), for a sample of independent uniforms over $(0, 1)$. The approximation is computed in a similar way as for `cramerVonMises`. To implement this method, a table of the values of $g(x) = \lim_{N\to\infty} P[G_N \le x]$ and of its derivative was first computed by numerical integration. For $x \le 1.5$, the method uses this table with cubic spline interpolation. For $x > 1.5$, it uses the empirical curve $g(x) = 1 - e^{19-20x}$. A correction of order $1/\sqrt{N}$, obtained empirically from 10^7 simulation runs with $N = 256$ and also implemented as an interpolation table with an exponential tail, is then added. The absolute error is estimated to be less than 0.01, 0.005, 0.002, 0.0008, 0.0005, 0.0005, 0.0005 for $N = 16$, 32, 64, 128, 256, 512, 1024, respectively.

```
@Deprecated
public static double andersonDarling (int N, double x)
```

Use `AndersonDarlingDistQuick.cdf(N, x)` instead. Returns $P[A_N^2 \le x]$, where A_N^2 is the Anderson-Darling statistic [2] defined in (23), for a sample of independent uniforms over $(0, 1)$. The approximation is computed similarly as for `cramerVonMises`. To implement this method, an interpolation table of the values of $g(x) = \lim_{N\to\infty} P[A_N^2 \le x]$ was first computed by numerical integration. Then a linear correction in $1/N$ obtained by simulation was added. The absolute error on $g_N(x)$ is estimated to be less than 0.001 for $N > 6$. For $N = 2$, 3, 4, 6, it is estimated to be less than 0.04, 0.01, 0.005, 0.002, respectively. For $N = 1$, the method returns the exact value, $g_N(x) = \sqrt{1 - 4e^{-x-1}}$ for $x \ge \ln(4) - 1$.

```
public static double scan (int N, double d, int m)
```

Returns $F(m)$, the distribution function of the scan statistic with parameters N and d, evaluated at m. For a description of this statistic and its distribution, see `scan`, which computes its complementary distribution $\bar{F}(m) = 1 - F(m - 1)$.

FBar

WARNING: All methods in this class are **deprecated**, except the method `scan`. They now call the method `barF` of the appropriate class in package `probdist`, which use better approximations than the ones that were previously used in this class.

This class is similar to `FDist`, except that it provides static methods to compute or approximate the complementary distribution function of X, which we define as $\bar{F}(x) = P[X \geq x]$, instead of $F(x) = P[X \leq x]$. Note that with our definition of $\bar{F}$, one has $\bar{F}(x) = 1 - F(x)$ for continuous distributions and $\bar{F}(x) = 1 - F(x-1)$ for discrete distributions over the integers. This is non-standard but we find it convenient.

For more details about the specific distributions, see the class `FDist`. When $F(x)$ is very close to 1, these methods generally provide much more precise values of $\bar{F}(x)$ than using $1 - F(x)$ where $F(x)$ is computed by a method from `FDist`.

```
package umontreal.iro.lecuyer.gof;

public class FBar
```

```
@Deprecated
public static double kolmogorovSmirnov (int n, double x)
```

Use `KolmogorovSmirnovDistQuick.barF(n, x)` instead. Returns $P[D_n > x]$, where D_n is the Kolmogorov-Smirnov statistic.

```
@Deprecated
public static double kolmogorovSmirnovPlus (int n, double x)
```

Use `KolmogorovSmirnovPlusDist.barF(n, x)` instead. Returns $P[D_n^+ > x]$, where D_n^+ is the Kolmogorov-Smirnov+ statistic.

```
@Deprecated
public static double cramerVonMises (int n, double x)
```

Use `CramerVonMisesDist.barF(n, x)` instead. Returns $P[W_n^2 > x]$, where W_n^2 is the Cramér-von Mises statistic.

```
@Deprecated
public static double watsonU (int n, double x)
```

Use `WatsonUDist.barF(n, x)` instead. Returns $P[U_n^2 > x]$, where U_n^2 is the Watson U statistic.

```
@Deprecated
public static double watsonG (int n, double x)
```

Use `WatsonGDist.barF(n, x)` instead. Returns $P[G_n > x]$, where G_n is the Watson G statistic.

```
@Deprecated
public static double andersonDarling (int n, double x)
```

Use `AndersonDarlingDistQuick.barF(n, x)` instead. Returns $P[A_n^2 > x]$, where A_n^2 is the Anderson-Darling statistic.

```
public static double scan (int n, double d, int m)
```

Return $P[S_N(d) \geq m]$, where $S_N(d)$ is the scan statistic(see [6, 7] and `scan`), defined as

$$S_N(d) = \sup_{0 \leq y \leq 1-d} \eta[y,\, y+d], \tag{15}$$

where d is a constant in $(0,1)$, $\eta[y,\, y+d]$ is the number of observations falling inside the interval $[y, y+d]$, from a sample of N i.i.d. $U(0,1)$ random variables. One has (see [1]),

$$P[S_N(d) \geq m] \approx \left(\frac{m}{d} - N - 1\right) b(m) + 2\sum_{i=m}^{N} b(i) \tag{16}$$

$$\approx 2(1 - \Phi(\theta\kappa)) + \theta\kappa \frac{\exp(-\theta^2\kappa^2/2)}{d\sqrt{2\pi}} \tag{17}$$

where Φ is the standard normal distribution function.

$$\begin{aligned} b(i) &= \binom{N}{i} d^i (1-d)^{N-i}, \\ \theta &= \sqrt{\frac{d}{1-d}}, \\ \kappa &= \frac{m}{d\sqrt{N}} - \sqrt{N}. \end{aligned}$$

For $d \leq 1/2$, (16) is exact for $m > N/2$, but only an approximation otherwise. The approximation (17) is good when Nd^2 is large or when $d > 0.3$ and $N > 50$. In other cases, this implementation sometimes use the approximation proposed by Glaz [6]. For more information, see [1, 6, 19]. The approximation returned by this function is generally good when it is close to 0, but is not very reliable when it exceeds, say, 0.4.

If $m \leq (N+1)d$, the method returns 1. Else, if $Nd \leq 10$, it returns the approximation given by Glaz [6]. If $Nd > 10$, it computes (17) or (16) and returns the result if it does not exceed 0.4, otherwise it computes the approximation from [6], returns it if it is less than 1.0, and returns 1.0 otherwise. The relative error can reach 10% when $Nd \leq 10$ or when the returned value is less than 0.4. For $m > Nd$ and $Nd > 10$, a returned value that exceeds 0.4 should be regarded as unreliable. For $m = 3$, the returned values are totally unreliable. (There may be an error in the original formulae in [6]).

Restrictions: $N \geq 2$ and $d \leq 1/2$.

GofStat

This class provides methods to compute several types of EDF goodness-of-fit test statistics and to apply certain transformations to a set of observations. This includes the probability integral transformation $U_i = F(X_i)$, as well as the power ratio and iterated spacings transformations [18]. Here, $U_{(0)}, \ldots, U_{(N-1)}$ stand for N observations $U_0, \ldots, U_{N-1}$ sorted by increasing order, where $0 \le U_i \le 1$.

Note: This class uses the Colt library.

```
package umontreal.iro.lecuyer.gof;

import cern.colt.list.*;


public class GofStat
```

Transforming the observations

```
public static DoubleArrayList unifTransform (DoubleArrayList data,
                                              ContinuousDistribution dist)
```

Applies the transformation $U_i = F(V_i)$ for $i = 0, 1, \ldots, N-1$, where F is a *continuous* distribution function, and returns the result as an array of length N. V represents the N observations contained in `data`, and U, the returned transformed observations. If `data` contains random variables from the distribution function `dist`, then the result will contain uniform random variables over $[0, 1]$.

```
public static DoubleArrayList unifTransform (DoubleArrayList data,
                                             DiscreteDistribution dist)
```

Applies the transformation $U_i = F(V_i)$ for $i = 0, 1, \ldots, N-1$, where F is a *discrete* distribution function, and returns the result as an array of length N. V represents the N observations contained in `data`, and U, the returned transformed observations.

Note: If V are the values of random variables with distribution function `dist`, then the result will contain the values of *discrete* random variables distributed over the set of values taken by `dist`, not uniform random variables over $[0, 1]$.

```
public static void diff (IntArrayList sortedData, IntArrayList spacings,
                         int n1, int n2, int a, int b)
```

Assumes that the real-valued observations $U_0, \ldots, U_{N-1}$ contained in `sortedData` are already sorted in increasing order and computes the differences between the successive observations. Let D be the differences returned in `spacings`. The difference $U_i - U_{i-1}$ is put in D_i for `n1 < i <= n2`, whereas $U_{n1} - a$ is put into D_{n1} and $b - U_{n2}$ is put into D_{n2+1}. The number of observations must be greater or equal than `n2`, we must have `n1 < n2`, and `n1` and `n2` are greater than 0. The size of `spacings` will be at least $N+1$ after the call returns.

```
public static void diff (DoubleArrayList sortedData,
                         DoubleArrayList spacings,
                         int n1, int n2, double a, double b)
```

Same as method `diff(IntArrayList,IntArrayList,int,int,int,int)`, but for the continuous case.

```
public static void iterateSpacings (DoubleArrayList data,
                                    DoubleArrayList spacings)
```

Applies one iteration of the *iterated spacings* transformation [9, 18]. Let U be the N observations contained into `data`, and let S be the spacings contained into `spacings`, Assumes that $S[0..N]$ contains the *spacings* between N real numbers $U_0, \ldots, U_{N-1}$ in the interval $[0, 1]$. These spacings are defined by

$$S_i = U_{(i)} - U_{(i-1)}, \qquad 1 \le i < N,$$

where $U_{(0)} = 0$, $U_{(N-1)} = 1$, and $U_{(0)}, \ldots, U_{(N-1)}$, are the U_i sorted in increasing order. These spacings may have been obtained by calling `diff`. This method transforms the spacings into new spacings, by a variant of the method described in section 11 of [14] and also by Stephens [18]: it sorts $S_0, \ldots, S_N$ to obtain $S_{(0)} \le S_{(1)} \le S_{(2)} \le \cdots \le S_{(N)}$, computes the weighted differences

$$\begin{aligned}
S_0 &= (N+1)S_{(0)}, \\
S_1 &= N(S_{(1)} - S_{(0)}), \\
S_2 &= (N-1)(S_{(2)} - S_{(1)}), \\
&\vdots \\
S_N &= S_{(N)} - S_{(N-1)},
\end{aligned}$$

and computes $V_i = S_0 + S_1 + \cdots + S_i$ for $0 \le i < N$. It then returns $S_0, \ldots, S_N$ in `S[0..N]` and $V_1, \ldots, V_N$ in `V[1..N]`.

Under the assumption that the U_i are i.i.d. $U(0, 1)$, the new S_i can be considered as a new set of spacings having the same distribution as the original spacings, and the V_i are a new sample of i.i.d. $U(0, 1)$ random variables, sorted by increasing order.

This transformation is useful to detect *clustering* in a data set: A pair of observations that are close to each other is transformed into an observation close to zero. A data set with unusually clustered observations is thus transformed to a data set with an accumulation of observations near zero, which is easily detected by the Anderson-Darling GOF test.

```
public static void powerRatios (DoubleArrayList sortedData)
```

Applies the *power ratios* transformation W described in section 8.4 of Stephens [18]. Let U be the N observations contained into `sortedData`. Assumes that U contains N real numbers $U_{(0)}, \ldots, U_{(N-1)}$ from the interval $[0, 1]$, already sorted in increasing order, and computes the transformations:

$$U'_i = (U_{(i)}/U_{(i+1)})^{i+1}, \qquad i = 0, \ldots, N-1,$$

with $U_{(N)} = 1$. These U'_i are sorted in increasing order and put back in `U[1...N]`. If the $U_{(i)}$ are i.i.d. $U(0, 1)$ sorted by increasing order, then the U'_i are also i.i.d. $U(0, 1)$.

This transformation is useful to detect clustering, as explained in `iterateSpacings`, except that here a pair of observations close to each other is transformed into an observation close to 1. An accumulation of observations near 1 is also easily detected by the Anderson-Darling GOF test.

Partitions for the chi-square tests

`public static class OutcomeCategoriesChi2`

This class helps managing the partitions of possible outcomes into categories for applying chi-square tests. It permits one to automatically regroup categories to make sure that the expected number of observations in each category is large enough. To use this facility, one must first construct an `OutcomeCategoriesChi2` object by passing to the constructor the expected number of observations for each original category. Then, calling the method `regroupCategories` will regroup categories in a way that the expected number of observations in each category reaches a given threshold `minExp`. Experts in statistics recommend that `minExp` be always larger than or equal to 5 for the chi-square test to be valid. Thus, `minExp` = 10 is a safe value to use. After the call, `nbExp` gives the expected numbers in the new categories and `loc[i]` gives the relocation of category i, for each i. That is, `loc[i] = j` means that category i has been merged with category j because its original expected number was too small, and `nbExp[i]` has been added to `nbExp[j]` and then set to zero. In this case, all observations that previously belonged to category i are redirected to category j. The variable `nbCategories` gives the final number of categories, `smin` contains the new index of the lowest category, and `smax` the new index of the highest category.

`public int nbCategories;`

Total number of categories.

`public int smin;`

Minimum index for valid expected numbers in the array `nbExp`.

`public int smax;`

Maximum index for valid expected numbers in the array `nbExp`.

`public double[] nbExp;`

Expected number of observations for each category.

`public int[] loc;`

`loc[i]` gives the relocation of the category `i` in the `nbExp` array.

`public OutcomeCategoriesChi2 (double[] nbExp)`

Constructs an `OutcomeCategoriesChi2` object using the array `nbExp` for the number of expected observations in each category. The `smin` and `smax` fields are set to 0 and $(n - 1)$ respectively, where n is the length of array `nbExp`. The `loc` field is set such that `loc[i]=i` for each `i`. The field `nbCategories` is set to n.

```
public OutcomeCategoriesChi2 (double[] nbExp, int smin, int smax)
```

Constructs an `OutcomeCategoriesChi2` object using the given `nbExp` expected observations array. Only the expected numbers from the `smin` to `smax` (inclusive) indices will be considered valid. The `loc` field is set such that `loc[i]=i` for each `i` in the interval `[smin, smax]`. All `loc[i]` for `i` $\le$ `smin` are set to `smin`, and all `loc[i]` for `i` $\ge$ `smax` are set to `smax`. The field `nbCategories` is set to (`smax - smin + 1`).

```
public OutcomeCategoriesChi2 (double[] nbExp, int[] loc,
                              int smin, int smax, int nbCat)
```

Constructs an `OutcomeCategoriesChi2` object. The field `nbCategories` is set to `nbCat`.

```
public void regroupCategories (double minExp)
```

Regroup categories as explained earlier, so that the expected number of observations in each category is at least `minExp`. We usually choose `minExp` $= 10$.

```
public String toString()
```

Provides a report on the categories.

Computing EDF test statistics

```
public static double chi2 (double[] nbExp, int[] count,
                           int smin, int smax)
```

Computes and returns the chi-square statistic for the observations o_i in `count[smin...smax]`, for which the corresponding expected values e_i are in `nbExp[smin...smax]`. Assuming that i goes from 1 to k, where k = `smax-smin+1` is the number of categories, the chi-square statistic is defined as

$$X^2 = \sum_{i=1}^{k} \frac{(o_i - e_i)^2}{e_i}. \tag{18}$$

Under the hypothesis that the e_i are the correct expectations and if these e_i are large enough, X^2 follows approximately the chi-square distribution with $k-1$ degrees of freedom. If some of the e_i are too small, one can use `OutcomeCategoriesChi2` to regroup categories.

```
public static double chi2 (IntArrayList data, DiscreteDistributionInt dist,
                           int smin, int smax, double minExp, int[] numCat)
```

Computes and returns the chi-square statistic for the observations stored in `data`, assuming that these observations follow the discrete distribution `dist`. For `dist`, we assume that there is one set $S = \{a, a+1, \ldots, b-1, b\}$, where $a < b$ and $a \ge 0$, for which $p(s) > 0$ if $s \in S$ and $p(s) = 0$ otherwise.

Generally, it is not possible to divide the integers in intervals satisfying $nP(a_0 \le s < a_1) = nP(a_1 \le s < a_2) = \cdots = nP(a_{j-1} \le s < a_j)$ for a discrete distribution, where n is the sample size, i.e., the number of observations stored into `data`. To perform a general chi-square test, the method starts from `smin` and finds the first non-negligible probability $p(s) \ge \epsilon$, where ϵ = `DiscreteDistributionInt.EPSILON`. It uses `smax` to allocate an array storing the number of expected observations ($np(s)$) for each $s \geq$ `smin`. Starting from $s =$ `smin`, the $np(s)$ terms are computed and the allocated array grows if required until a negligible probability term is found. This gives the number of expected elements for each category, where an outcome category corresponds here to an interval in which sample observations could lie. The categories are regrouped to have at least `minExp` observations per category. The method then counts the number of samples in each categories and calls `chi2` to get the chi-square test statistic. If `numCat` is not `null`, the number of categories after regrouping is returned in `numCat[0]`. The number of degrees of freedom is equal to `numCat[0]-1`. We usually choose `minExp` $= 10$.

```
public static double chi2Equal (double nbExp, int[] count,
                                int smin, int smax)
```

Similar to `chi2`, except that the expected number of observations per category is assumed to be the same for all categories, and equal to `nbExp`.

```
public static double chi2Equal (DoubleArrayList data, double minExp)
```

Computes the chi-square statistic for a continuous distribution. Here, the equiprobable case can be used. Assuming that `data` contains observations coming from the uniform distribution, the $[0, 1]$ interval is divided into $1/p$ subintervals, where $p =$ `minExp`$/n$, n being the sample size, i.e., the number of observations stored in `data`. For each subinterval, the method counts the number of contained observations and the chi-square statistic is computed using `chi2Equal`. We usually choose `minExp` $= 10$.

```
public static double chi2Equal (DoubleArrayList data)
```

Equivalent to `chi2Equal (data, 10)`.

```
public static int scan (DoubleArrayList sortedData, double d)
```

Computes and returns the scan statistic $S_N(d)$, defined in (15). Let U be the N observations contained into `sortedData`. The N observations in $U[0..N-1]$ must be real numbers in the interval $[0, 1]$, sorted in increasing order. (See `FBar.scan` for the distribution function of $S_N(d)$).

```
public static double cramerVonMises (DoubleArrayList sortedData)
```

Computes and returns the Cramér-von Mises statistic W_N^2 (see [5, 16, 17]), defined by

$$W_N^2 = \frac{1}{12N} + \sum_{j=0}^{N-1} \left(U_{(j)} - \frac{(j+0.5)}{N} \right)^2, \tag{19}$$

assuming that `sortedData` contains $U_{(0)}, \ldots, U_{(N-1)}$ sorted in increasing order.

```
public static double watsonG (DoubleArrayList sortedData)
```

Computes and returns the Watson statistic G_N (see [20, 4]), defined by

$$\begin{aligned} G_N &= \sqrt{N} \max_{0 \leq j \leq N-1} \left\{ (j+1)/N - U_{(j)} + \overline{U}_N - 1/2 \right\} \qquad (20) \\ &= \sqrt{N} \left(D_N^+ + \overline{U}_N - 1/2 \right), \end{aligned}$$

where $\overline{U}_N$ is the average of the observations $U_{(j)}$, assuming that `sortedData` contains the sorted $U_{(0)}, \ldots, U_{(N-1)}$.

`public static double watsonU (DoubleArrayList sortedData)`

Computes and returns the Watson statistic U_N^2 (see [5, 16, 17]), defined by

$$W_N^2 = \frac{1}{12N} + \sum_{j=0}^{N-1} \left\{ U_{(j)} - \frac{(j+0.5)}{N} \right\}^2, \tag{21}$$

$$U_N^2 = W_N^2 - N\left(\overline{U}_N - 1/2\right)^2. \tag{22}$$

where $\overline{U}_N$ is the average of the observations $U_{(j)}$, assuming that `sortedData` contains the sorted $U_{(0)}, \ldots, U_{(N-1)}$.

`public static double EPSILONAD = Num.DBL_EPSILON / 2.0;`

Used by `andersonDarling`.

`public static double andersonDarling (DoubleArrayList sortedData)`

Computes and returns the Anderson-Darling statistic A_N^2 (see [13, 17, 2]), defined by

$$A_N^2 = -N - \frac{1}{N} \sum_{j=0}^{N-1} \left\{ (2j+1)\ln(U_{(j)}) + (2N-1-2j)\ln(1-U_{(j)}) \right\},$$

assuming that `sortedData` contains $U_{(0)}, \ldots, U_{(N-1)}$.

When computing A_N^2, all observations U_i are projected to the interval $[\epsilon, 1-\epsilon]$ for some $\epsilon > 0$, in order to avoid numerical overflow when taking the logarithm of U_i or $1 - U_i$. The variable `EPSILONAD` gives the value of ϵ. `Num.DBL_EPSILON` is usually 2^{-52}.

`public static double[] kolmogorovSmirnov (DoubleArrayList sortedData)`

Computes the Kolmogorov-Smirnov (KS) test statistics D_N^+, D_N^-, and D_N defined by

$$D_N^+ = \max_{0 \le j \le N-1} \left((j+1)/N - U_{(j)}\right), \tag{23}$$

$$D_N^- = \max_{0 \le j \le N-1} \left(U_{(j)} - j/N\right), \tag{24}$$

$$D_N = \max\,(D_N^+, D_N^-). \tag{25}$$

and returns an array of length 3 that contains their values at positions 0, 1, and 2, respectively.

These statistics compare the empirical distribution of $U_{(1)}, \ldots, U_{(N)}$, which are assumed to be in `sortedData`, with the uniform distribution.

```
public static double[] kolmogorovSmirnovJumpOne (DoubleArrayList sortedData,
                                                  double a)
```

Compute the KS statistics $D_N^+(a)$ and $D_N^-(a)$ defined in the description of the method `FDist.kolmogorovSmirnovPlusJumpOne`, assuming that F is the uniform distribution over $[0, 1]$

and that $U_{(1)}, \ldots, U_{(N)}$ are in `sortedData`. Returns an array of length 2 that contains their values at positions 0 and 1, respectively.

`public static double pDisc (double pL, double pR)`

Computes a variant of the p-value p whenever a test statistic has a *discrete* probability distribution. This p-value is defined as follows:

$$\begin{aligned} p_L &= P[Y \le y] \\ p_R &= P[Y \ge y] \\ p &= \begin{cases} p_R, & \text{if } p_R < p_L \\ 1 - p_L, & \text{if } p_R \ge p_L \text{ and } p_L < 0.5 \\ 0.5 & \text{otherwise.} \end{cases} \end{aligned}$$

The function takes p_L and p_R as input and returns p.

GofFormat

This class contains methods used to format results of GOF test statistics, or to apply a series of tests simultaneously and format the results. It is in fact a translation from C to Java of a set of functions that were specially written for the implementation of TestU01, a software package for testing uniform random number generators [12].

Strictly speaking, applying several tests simultaneously makes the p-values "invalid" in the sense that the probability of having *at least one* p-value less than 0.01, say, is larger than 0.01. One must therefore be careful with the interpretation of these p-values (one could use, e.g., the Bonferroni inequality [11]). Applying simultaneous tests is convenient in some situations, such as in screening experiments for detecting statistical deficiencies in random number generators. In that context, rejection of the null hypothesis typically occurs with extremely small p-values (e.g., less than 10^{-15}), and the interpretation is quite obvious in this case.

The class also provides tools to plot an empirical or theoretical distribution function, by creating a data file that contains a graphic plot in a format compatible with the software specified by the environment variable `graphSoft`.

Note: This class uses the Colt library.

```
package umontreal.iro.lecuyer.gof;

public class GofFormat
```

Plotting distribution functions

```
public static final int GNUPLOT
```

Data file format used for plotting functions with Gnuplot.

```
public static final int MATHEMATICA
```

Data file format used for creating graphics with Mathematica.

```
public static int graphSoft = GNUPLOT;
```

Environment variable that selects the type of software to be used for plotting the graphs of functions. The data files produced by `graphFunc` and `graphDistUnif` will be in a format suitable for this selected software. The default value is `GNUPLOT`. To display a graphic in file `f` using `gnuplot`, for example, one can use the command "`plot f with steps, x with lines`" in `gnuplot`.

```
@Deprecated
public static String graphFunc (ContinuousDistribution dist, double a,
                                double b, int m, int mono, String desc)
```

Use `drawCdf` instead. Formats data to plot the graph of the distribution function F (or $\bar{F}$) over the interval $[a, b]$, and returns the result as a `String`. `dist.cdf(x)` (or `dist.barF(x)`) returns the value of F (or $\bar{F}$) at x, and that F is either non-decreasing or non-increasing. If `mono` $= 1$, the method will verify that F is non-decreasing; if `mono` $= -1$, it will verify that $\bar{F}$ is non-increasing. (This is useful to verify if F is effectively a sensible approximation to a distribution function or its complementary in the given interval.) The `String desc` gives a short caption for the graphic plot. The method computes the $m + 1$ points $(x_i,\, F(x_i))$, where $x_i = a + i(b - a)/m$ for $i = 0, 1, \ldots, m$, and formats these points into a `String` in a format suitable for the software specified by `graphSoft`.

```
public static String drawCdf (ContinuousDistribution dist, double a,
                              double b, int m, String desc)
```

Formats data to plot the graph of the distribution function F over the interval $[a, b]$, and returns the result as a `String`. The method `dist.cdf(x)` returns the value of F at x. The `String desc` gives a short caption for the graphic plot. The method computes the $m + 1$ points $(x_i,\, F(x_i))$, where $x_i = a + i(b - a)/m$ for $i = 0, 1, \ldots, m$, and formats these points into a `String` in a format suitable for the software specified by `graphSoft`.

```
public static String drawDensity (ContinuousDistribution dist, double a,
                                  double b, int m, String desc)
```

Formats data to plot the graph of the density $f(x)$ over the interval $[a, b]$, and returns the result as a `String`. The method `dist.density(x)` returns the value of $f(x)$ at x. The `String desc` gives a short caption for the graphic plot. The method computes the $m + 1$ points $(x_i,\, f(x_i))$, where $x_i = a + i(b - a)/m$ for $i = 0, 1, \ldots, m$, and formats these points into a `String` in a format suitable for the software specified by `graphSoft`.

```
public static String graphDistUnif (DoubleArrayList data, String desc)
```

Formats data to plot the empirical distribution of $U_{(1)}, \ldots, U_{(N)}$, which are assumed to be in `data[0...N-1]`, and to compare it with the uniform distribution. The $U_{(i)}$ must be sorted. The two endpoints $(0, 0)$ and $(1, 1)$ are always included in the plot. The string `desc` gives a short caption for the graphic plot. The data is printed in a format suitable for the software specified by `graphSoft`.

Computing and printing p-values for EDF test statistics

```
public static double EPSILONP = 1.0E-15;
```

Environment variable used in `formatp0` to determine which p-values are too close to 0 or 1 to be printed explicitly. If `EPSILONP` $= \epsilon$, then any p-value (or significance level) less than ϵ or larger than $1 - \epsilon$ is *not* written explicitly; the program simply writes "`eps`" or "`1-eps`". The default value is 10^{-15}.

```
public static double SUSPECTP = 0.01;
```

Environment variable used in `formatp1` to determine which p-values should be marked as suspect when printing test results. If `SUSPECTP` $= \alpha$, then any p-value (or significance level) less than α or larger than $1 - \alpha$ is considered suspect and is "singled out" by `formatp1`. The default value is 0.01.

```
public static String formatp0 (double p)
```

Returns the significance level (or p-value) p of a test, in the format "$1 - p$" if p is close to 1, and p otherwise. Uses the environment variable `EPSILONP` and replaces p by ϵ when it is too small.

```
public static String formatp1 (double p)
```

Returns the string "`Significance level of test : `", then calls `formatp0` to print p, and adds the marker "`****`" if p is considered suspect (uses the environment variable `RSUSPECTP` for this).

```
public static String formatp2 (double x, double p)
```

Returns `x` on a single line, then go to the next line and calls `formatp1`.

```
public static String formatp3 (String testName, double x, double p)
```

Formats the test statistic `x` for a test named `testName` with p-value `p`. The first line of the returned string contains the name of the test and the statistic whereas the second line contains its significance level. The formated values of `x` and `p` are aligned.

```
public static String formatChi2 (int k, int d, double chi2)
```

Computes the p-value of the chi-square statistic `chi2` for a test with `k` intervals. Uses d decimal digits of precision in the calculations. The result of the test is returned as a string. The p-value is computed using `pDisc`.

```
public static String formatKS (int n, double dp,
                               double dm, double d)
```

Computes the p-values of the three Kolmogorov-Smirnov statistics D_N^+, D_N^-, and D_N, whose values are in `dp, dm, d`, respectively, assuming a sample of size `n`. Then formats these statistics and their p-values using `formatp2` for each one.

```
public static String formatKS (DoubleArrayList data,
                               ContinuousDistribution dist)
```

Computes the KS test statistics to compare the empirical distribution of the observations in `data` with the theoretical distribution `dist` and formats the results.

```
public static String formatKSJumpOne (int n, double a, double dp)
```

Similar to `formatKS`, but for the KS statistic $D_N^+(a)$ defined in (10). Writes a header, computes the p-value and calls `formatp2`.

```
public static String formatKSJumpOne (DoubleArrayList data,
                                      ContinuousDistribution dist,
                                      double a)
```

Similar to `formatKS`, but for $D_N^+(a)$ defined in (10).

Applying several tests at once and printing results

Higher-level tools for applying several EDF goodness-of-fit tests simultaneously are offered here. The environment variable `activeTests` specifies which tests in this list are to be performed when asking for several simultaneous tests via the functions `activeTests`, `formatActiveTests`, etc.

`public  static final int KSP = 0;`

Kolmogorov-Smirnov+ test

`public static final int KSM = 1;`

Kolmogorov-Smirnov− test

`public static final int KS = 2;`

Kolmogorov-Smirnov test

`public static final int AD = 3;`

Anderson-Darling test

`public static final int CM = 4;`

Cramér-von Mises test

`public static final int WG = 5;`

Watson G test

`public static final int WU = 6;`

Watson U test

`public static final int MEAN = 7;`

Mean

`public static final int COR = 8;`

Correlation

`public static final int NTESTTYPES = 9;`

Total number of test types

`public static final String[] TESTNAMES`

Name of each `testType` test. Could be used for printing the test results, for example.

`public static boolean[] activeTests`

The set of EDF tests that are to be performed when calling the methods `activeTests`, `formatActiveTests`, etc. By default, this set contains `KSP`, `KSM`, and `AD`. Note: `MEAN` and `COR` are *always excluded* from this set of active tests.

`public static void tests (DoubleArrayList sortedData, double[] sVal)`

Computes all EDF test statistics enumerated above (except `COR`) to compare the empirical distribution of $U_{(0)}, \dots, U_{(N-1)}$ with the uniform distribution, assuming that these sorted observations are in `sortedData`. If $N > 1$, returns `sVal` with the values of the KS statistics D_N^+, D_N^- and D_N, of the Cramér-von Mises statistic W_N^2, Watson's G_N and U_N^2, Anderson-Darling's A_N^2, and the average of the U_i's, respectively. If $N = 1$, only puts $1-$`sortedData.get (0)` in `sVal[KSP]`. Calling this method is more efficient than computing these statistics separately by calling the corresponding methods in `GofStat`.

```
public static void tests (DoubleArrayList data,
                          ContinuousDistribution dist, double[] sVal)
```

The observations V are in `data`, not necessarily sorted, and their empirical distribution is compared with the continuous distribution `dist`. If $N = 1$, only puts `data.get (0)` in `sVal[MEAN]`, and $1 -$ `dist.cdf (data.get (0))` in `sVal[KSP]`.

```
public static void activeTests (DoubleArrayList sortedData,
                                double[] sVal, double[] pVal)
```

Computes the EDF test statistics by calling `tests`, then computes the p-values of those that currently belong to `activeTests`, and return these quantities in `sVal` and `pVal`, respectively. Assumes that $U_{(0)}, \ldots, U_{(N-1)}$ are in `sortedData` and that we want to compare their empirical distribution with the uniform distribution. If $N = 1$, only puts $1 -$ `sortedData.get (0)` in `sVal[KSP], pVal[KSP]`, and `pVal[MEAN]`.

```
public static void activeTests (DoubleArrayList data,
                                ContinuousDistribution dist,
                                double[] sVal, double[] pVal)
```

The observations are in `data`, not necessarily sorted, and we want to compare their empirical distribution with the distribution `dist`. If $N = 1$, only puts `data.get(0)` in `sVal[MEAN]`, and $1 -$ `dist.cdf (data.get (0))` in `sVal[KSP], pVal[KSP]`, and `pVal[MEAN]`.

```
public static String formatActiveTests (int n, double[] sVal,
                                        double[] pVal)
```

Gets the p-values of the *active* EDF test statistics, which are in `activeTests`. It is assumed that the values of these statistics and their p-values are *already computed*, in `sVal` and `pVal`, and that the sample size is `n`. These statistics and p-values are formated using `formatp2` for each one. If `n=1`, prints only `pVal[KSP]` using `formatp1`.

```
public static String iterSpacingsTests (DoubleArrayList sortedData, int k,
                                        boolean printval, boolean graph,
                                        PrintWriter f)
```

Repeats the following `k` times: Applies the `GofStat.iterateSpacings` transformation to the $U_{(0)}, \ldots, U_{(N-1)}$, assuming that these observations are in `sortedData`, then computes the EDF test statistics and calls `activeTests` after each transformation. The function returns the *original* array `sortedData` (the transformations are applied on a copy of `sortedData`). If `printval = true`, stores all the values into the returned `String` after each iteration. If `graph = true`, calls `graphDistUnif` after each iteration to print to stream `f` the data for plotting the distribution function of the U_i.

```
public static String iterPowRatioTests (DoubleArrayList sortedData, int k,
                                        boolean printval, boolean graph,
                                        PrintWriter f)
```

Similar to `iterSpacingsTests`, but with the `GofStat.powerRatios` transformation.

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