Input Modeling Using a Computer Algebra System

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Introduction

- Fitting standard univariate parametric probability distributions with an input modeling package.
  - Typically fits several distributions to a data set
  - Uses goodness-of-fit statistics to determine the distribution with the best fit
  - What if an appropriate input model is not part of the package?
- Using a prototype Maple-based probability language, known as APPL (A Probability Programming Language) for input modeling. This language allows an analyst to:
  - Specify a standard or non-standard distribution for an input model and have derivations performed automatically
  - Compute parameter estimates
  - Plot empirical and fitted CDFs
  - Perform goodness-of-fit tests

About APPL

APPL's data structures and algorithms were initially developed to solve probability problems.

- Finds the distribution of
  - Order statistics
  - The sum of independent random variables
  - The product of independent random variables
  - The transformation of a random variable
  - Mixtures of random variables
- Calculates
  - Cumulative distribution functions
  - Expected values
  - Quantiles of a distribution
  - Maximum likelihood estimators

Probability theory examples using APPL

Example 1. $X_1, X_2, \ldots, X_8$ iid U(0, 1). Find

$$\Pr\left(\frac{7}{2} < \sum_{i=1}^{8} X_i < \frac{11}{2}\right)$$

The two standard methods for *approximating* the probability:

- Central limit theorem: only yields one digit of accuracy for this particular problem
- Monte Carlo simulation
  - requires custom coding
  - needs 100-fold increase in computation time for next additional digit of accuracy

The APPL statements

```
n := 8;
X := UniformRV(0, 1);
Y := ConvolutionIID(X, n);
CDF(Y, 11 / 2) - CDF(Y, 7 / 2);
```

yield the exact solution

$$\frac{3580151}{5160960}$$

This may be coded up more compactly as

```
Y := ConvolutionIID(UniformRV(0, 1), 8);
CDF(Y, 11 / 2) - CDF(Y, 7 / 2);
```

Example 2. $X \sim triangular(1, 2, 3)$ and $Y \sim U(1, 2)$. Assume X and Y are independent. Find the distribution of $V = XY$.

The APPL statements

```
X := TriangularRV(1, 2, 3);
Y := UniformRV(1, 2);
V := Product(X, Y);
```

return the PDF of `V` as

$$f_V(v) = \begin{cases} v - \ln(v) - 1 & 1 < v \le 2 \\ -\frac{3}{2}v + 4\ \ln(v) + 4 - 5\ \ln(2) & 2 < v \le 3 \\ -\frac{1}{2}\, v + \ln(\frac{27}{32}\, v) + 1 & 3 < v \le 4 \\ \frac{1}{2}\, v - 3\ \ln(v) - 3 + \ln(216) & 4 < v < 6. \end{cases}$$

Example 3. Let X be a random variable with the distribution associated with the Kolmogorov–Smirnov test statistic in the all parameters known case for sample size $n = 5$. Let Y be a Kolmogorov–Smirnov random variable with $n = 3$. If X and Y are independent, find $\text{Var}\left[\max\{X, Y\}\right]$.

The APPL statements

```
X := KSRV(5);
Y := KSRV(3);
Z := Maximum(X, Y);
Variance(Z);
```

yield

$$\frac{1036875145231938755837167 1}{667392326753906250000000000}$$

or approximately 0.0155362

Example 4. Let $X \sim triangular(a, b, c)$. Find the CDF of X.

The APPL statements

```
X := TriangularRV(a, b, c);
CDF(X);
```

yield the CDF of X as

$$F(x) = \begin{cases} 0 & x \le a \\ \dfrac{(x-a)^2}{(c-a)(b-a)} & a < x \le b \\ 1 - \dfrac{(c-x)^2}{(c-a)(c-b)} & b < x \le c \\ 1 & x > c \end{cases}$$

Example 5. $X_1, X_2, \ldots, X_7 \sim Weibull(\frac{1}{2}, 2)$ with PDF

$$f_X(x) = \frac{1}{2} x e^{-\frac{1}{4}x^2} \qquad x > 0.$$

Calculate the mean of the second order statistic.

The APPL statements

```
X := WeibullRV(1 / 2, 2);
Y := OrderStat(X, 7, 2);
Mean(Y);
```

return the mean of the second order statistic as

$$\frac{7}{6}\sqrt{6\pi} - \frac{6}{7}\sqrt{7\pi} \cong 1.0456613$$

Example 6. $X \sim geometric(\frac{1}{4})$ with PDF $f_X(x) = \frac{1}{4} \cdot \frac{3}{4}^{x-1}$, $x = 1, 2, \ldots$. Calculate the median of the maximum order statistic when $n = 5$ items are sampled *with replacement*.

The APPL statements

```
X := GeometricRV(1 / 4);
Y := OrderStat(X, 5, 5);
IDF(Y, 0.5);
```

return the median of the distribution as 8

Example 7. Let the random variable T have hazard function

$$h_T(t) = \begin{cases} \lambda & 0 < t < 1 \\ \lambda t & t \geq 1 \end{cases}$$

for $\lambda > 0$. Find the survivor function $S(t) = \Pr(T \geq t)$.

Input the hazard function for T as a list of three sublists:

```
assume(lambda > 0);
T := [[t -> lambda, t -> lambda * t],
      [0, 1, infinity],
      [`Continuous`, `HF`]];
SF(T);
```

The survivor function is returned as

$$S_T(t) = \begin{cases} e^{-\lambda t} & 0 < t < 1 \\ e^{-\lambda(t^2+1)/2} & t \geq 1 \end{cases}$$

Example 8. (Hogg and Craig, 1995, page 287) Let X_1 and X_2 be iid observations drawn from a population with PDF

$$f(x) = \theta x^{\theta - 1} \qquad\qquad 0 < x < 1,$$

where $\theta > 0$. Test H_0: $\theta = 1$ versus H_1: $\theta > 1$ using the test statistic $X_1 X_2$ and the critical region $C = \{(X_1, X_2) | X_1 X_2 \geq 3/4\}$. Find the significance level α and power function for the test.

The APPL statements to compute the power function are

```
n := 2;
crit := 3 / 4;
assume(theta > 0);
X := [[x -> theta * x ^ (theta - 1)],
      [0, 1], ['Continuous', 'PDF']];
T := ProductIID(X, n);
power := SF(T, crit);
```

which yields

$$\Pr(\text{rejecting } \; H_0 | \theta) = 1 - (3/4)^{\theta} + \theta (3/4)^{\theta} \ln(3/4)$$

The significance level of the test is computed with the statement

```
alpha := subs(theta = 1, power);
```

The result is $\alpha = 1/4 + 3/4 \ln(3/4) \cong 0.0342$

Plotting the power function requires the additional statement

```
plot(power, theta = 0 .. 4);
```

Example 9. Let $U_1 \sim U(0,1)$ and $U_2 \sim U(0,1)$. The Box–Muller algorithm for generating a single standard normal deviate V can be coded in one line (Devroye, 1996) as

$$V \leftarrow \sqrt{-2\ln U_1}\cos(2\pi U_2),$$

where U_1 and U_2 are independent random numbers.

The PDF of V, shown below, is computed with the statements:

```
U1 := UniformRV(0, 1);
U2 := UniformRV(0, 1);
g1 := [[x -> ln(x)], [0, infinity]];
X1 := Transform(U1, g1);
g2 := [[x -> -2 * x], [-infinity, infinity]];
X2 := Transform(X1, g2);
g3 := [[x -> sqrt(x)], [0, infinity]];
X3 := Transform(X2, g3);
h1 := [[x -> Pi * x], [-infinity, infinity]];
Y1 := Transform(U2, h1);
h2 := [[x -> cos(x)], [-infinity, infinity]];
Y2 := Transform(Y1, h2);
V := Product(X3, Y2);
```

$$h(v) = \begin{cases} \dfrac{v}{\pi}\displaystyle\int_{-1}^{0} \frac{e^{-v^2/(2x^2)}}{x^2\sqrt{1-x^2}}\,dx & -\infty < v < 0 \\ \dfrac{v}{\pi}\displaystyle\int_{0}^{1} \frac{e^{-v^2/(2x^2)}}{x^2\sqrt{1-x^2}}\,dx & 0 < v < \infty \end{cases}$$

This form is mathematically equivalent to

$$h(v) = \frac{1}{\sqrt{2\pi}} e^{-v^2/2} \qquad -\infty < v < \infty$$

Example 10. Use the K–S test for assessing model adequacy (goodness-of-fit) for the prime modulus multiplicative linear congruential random number generator:

$$z_{i+1} = az_i \mod m$$

for $i = 0, 1, \ldots$, where z_0 is a seed, $a = 7^5 = 16,807$, and $m = 2^{31} - 1 = 2,147,483,647$ (Park and Miller, 1988).

If the seed $z_0 = 987,654,321$ is used, the first five random numbers generated are

$$\frac{1,605,065,384}{2,147,483,647} \qquad \frac{1,791,818,921}{2,147,483,647} \qquad \frac{937,423,366}{2,147,483,647}$$

$$\frac{1,334,477,970}{2,147,483,647} \qquad \frac{252,032,522}{2,147,483,647}$$

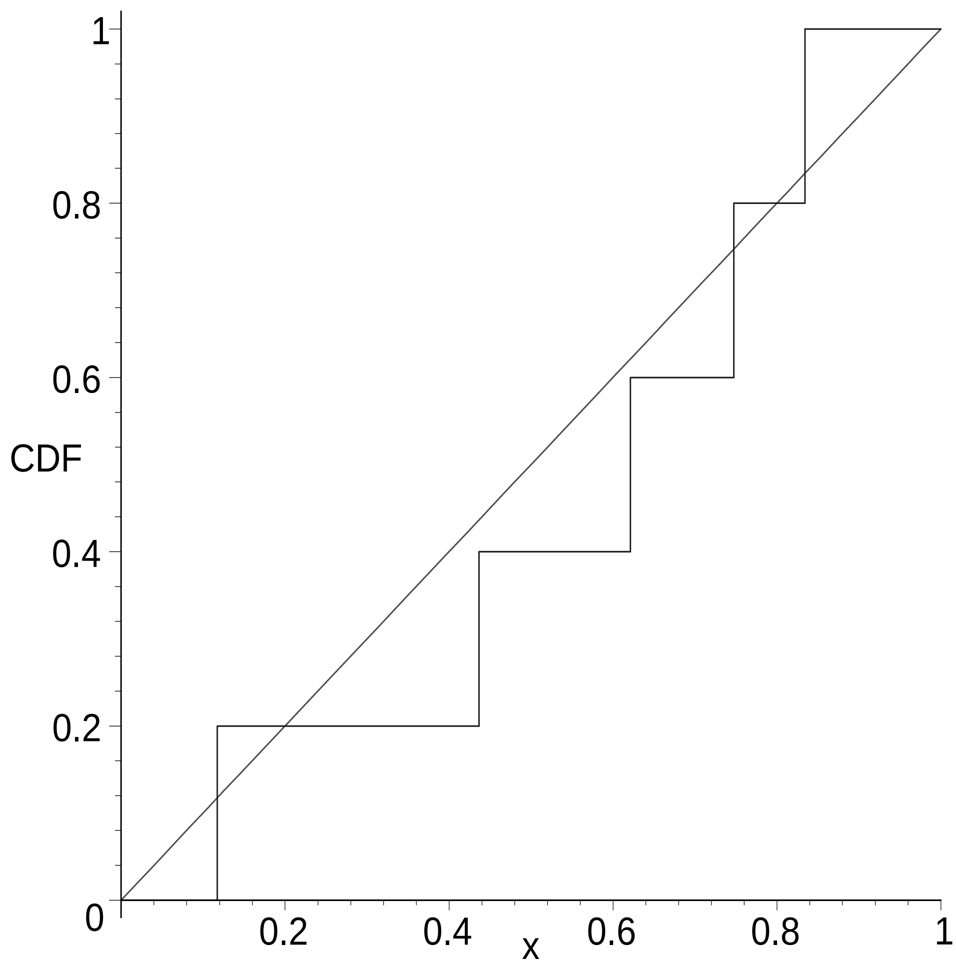
or, approximately

$$0.7474168 \qquad 0.8343807 \qquad 0.4365218$$

$$0.6214147 \qquad 0.1173618$$

Let `Sample` contain the five random numbers generated above. The APPL statements required to plot the empirical CDF of `Sample` and the theoretical U(0, 1) CDF are

```
n := 5; a := 7 ^ 5;
seed := 987654321; m := 2 ^ 31 - 1;
Sample := [];
for j from 1 to n do
  seed := a * seed mod m:
  Sample := [op(Sample), seed / m]:
od;
U := UniformRV(0, 1)
PlotEmpVsFittedCDF(U, Sample, [], 0, 1);
```



The Empirical CDF of `Sample` and the Theoretical U(0, 1) CDF

Let $F(x)$ be the hypothesized CDF and $F_5(x)$ be the empirical CDF. The Kolmogorov–Smirnov test statistic,

$$D_5 = \sup_x |F(x) - F_5(x)|,$$

is computed with the statement

```
TestStat := KSTest(U, Sample, []);
```

The approximate value of the test statistic for the five random numbers is 0.2365.

Since large values of the test statistic indicate a poor fit and the CDF $F_{D_5}(y)$ of the test statistic is (Drew, Glen and Leemis, 2000)

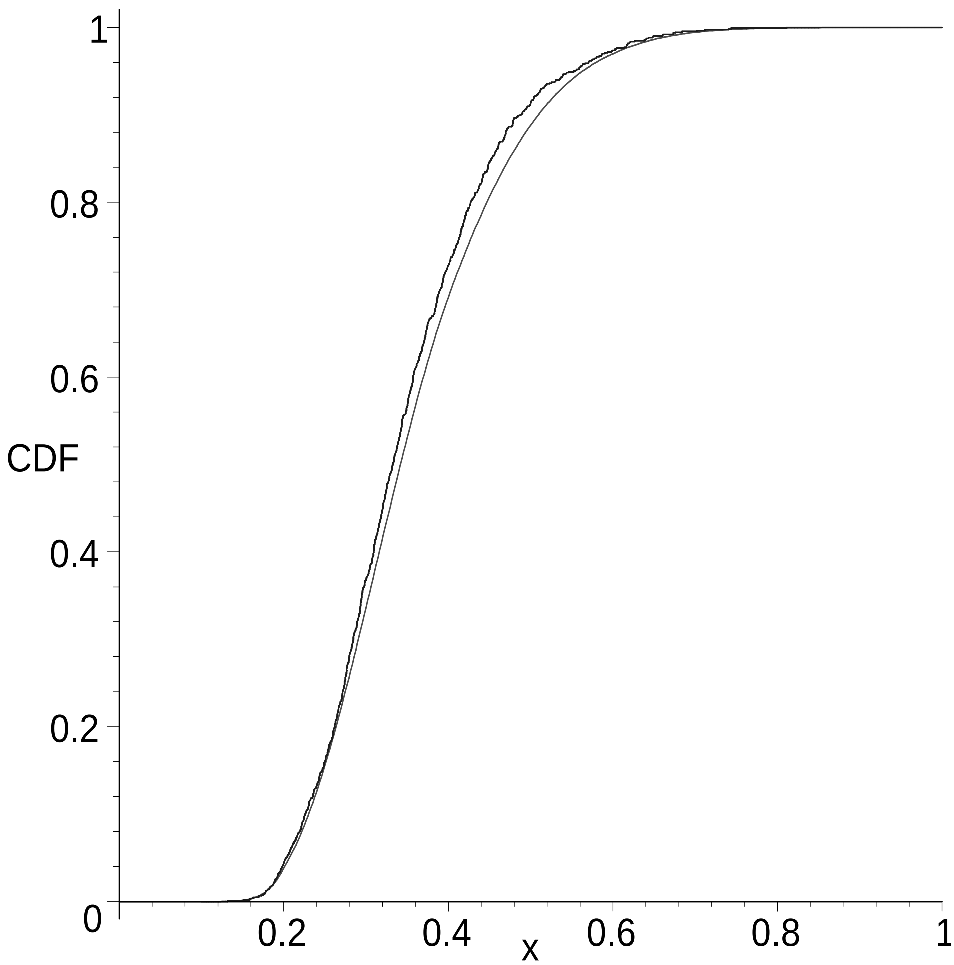
$$\begin{cases} 0 & y < \frac{1}{10} \\ \frac{24}{625}\,(10\,x-1)^5 & \frac{1}{10} \le y < \frac{1}{5} \\ -288\,x^4 + 240\,x^3 - \frac{1464}{25}\,x^2 + \frac{672}{125}\,x - \frac{96}{625} & \frac{1}{5} \le y < \frac{3}{10} \\ 160\,x^5 - 240\,x^4 + \frac{424}{5}\,x^3 + 12\,x^2 - \frac{168}{25}\,x + \frac{336}{625} & \frac{3}{10} \le y < \frac{2}{5} \\ -20\,x^5 + 74\,x^4 - \frac{456}{5}\,x^3 + \frac{224}{5}\,x^2 - \frac{728}{125}\,x & \frac{2}{5} \le y < \frac{1}{2} \\ 12\,x^5 - 6\,x^4 - \frac{56}{5}\,x^3 + \frac{24}{5}\,x^2 + \frac{522}{125}\,x - 1 & \frac{1}{2} \le y < \frac{3}{5} \\ -20\,y^6 + 32\,y^5 - \frac{185}{9}\,y^3 + \frac{175}{36}\,y^2 + \frac{3371}{648}\,y - 1 & \frac{1}{2} \le y < \frac{3}{5} \\ -8\,x^5 + 22\,x^4 - \frac{92}{5}\,x^3 + \frac{12}{25}\,x^2 + \frac{738}{125}\,x - 1 & \frac{3}{5} \le y < \frac{4}{5} \\ 2\,x^5 - 10\,x^4 + 20\,x^3 - 20\,x^2 + 10\,x - 1 & \frac{4}{5} \le y < 1 \\ 1 & y \ge 1, \end{cases}$$

the p-value for this particular test is found with the APPL statement

```
p := SF(KSRV(5), TestStat);
```

which yields $p \cong 0.8838$.

If this process is repeated for a total of 1000 groups of nonoverlapping consecutive sets of five random numbers, the empirical CDF of the K–S statistics should be close to the theoretical if the random number generator is valid.



Empirical CDF of 1000 Kolmogorov–Smirnov Statistics and the Theoretical Kolmogorov–Smirnov CDF for $n = 5$

Input Modeling

Maple and APPL can easily be adapted for use in input modeling.

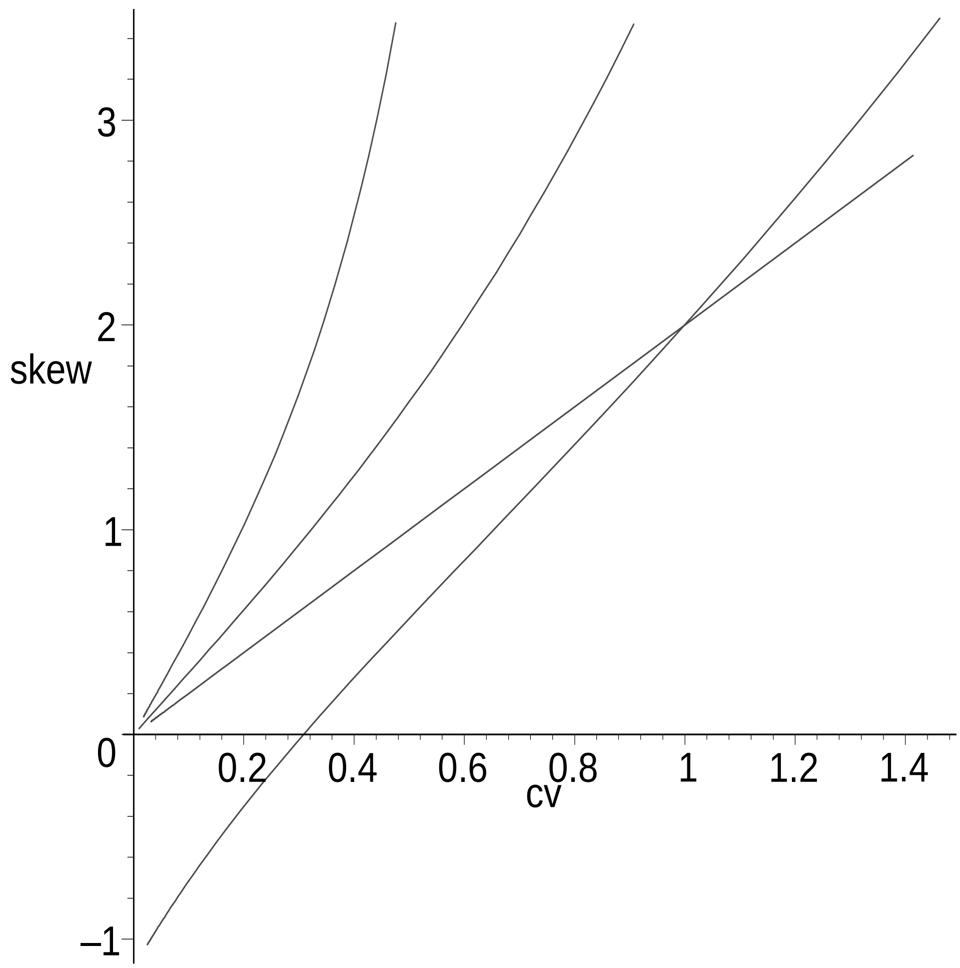
Example 11. *Model selection.* One of the tools for selecting a suitable input model is a plot of the coefficient of variation ($\gamma = \sigma/\mu$) versus the skewness

$$\gamma_3 = E\left[\left(\frac{X-\mu}{\sigma}\right)^3\right].$$

After constructing this plot, the sample coefficient of variance and sample skewness can be plotted for a particular data set to determine an appropriate distribution for modeling the data.

The statements necessary to plot the gamma distribution's coefficient of variation versus skewness are shown below. The plots for the other distributions are calculated similarly. The Maple statement used to display all four plots in one graphic is also provided.

```
unassign('kappa');  lambda := 1;
X := GammaRV(lambda, kappa);
c := CoefOfVar(X);
s := Skewness(X);
GammaPlot := plot([c, s, kappa = 0.5 .. 999],
    labels = [cv, skew]):
    .
    .
    .
plots[display]({GammaPlot, WeibullPlot,
    LogNormalPlot, LogLogisticPlot},
    scaling = unconstrained);
```



Coefficient of Variation, γ, Versus Skewness, γ_3, for the Gamma, Weibull, Log Normal, and Log Logistic Distributions

Example 12. The following $n = 23$ service times were collected to determine an input model in a discrete-event simulation of a queuing system. The service times in seconds are

$$
\begin{array}{cccccc}
105.84 & 28.92 & 98.64 & 55.56 & 128.04 & 45.60 \\
67.80 & 105.12 & 48.48 & 51.84 & 173.40 & 51.96 \\
54.12 & 68.64 & 93.12 & 68.88 & 84.12 & 68.64 \\
41.52 & 127.92 & 42.12 & 17.88 & 33.00. &
\end{array}
$$

[These service times are actually ball bearing failure times borrowed from the life testing literature (Lawless 1982, page 228)]

Consider fitting an exponential distribution to this data set using maximum likelihood. The data set, `BallBearing`, is pre-defined in APPL. The APPL statements

```
X := ExponentialRV(lambda);
lamhat := MLE(X, BallBearing, [lambda]);
```

return $\hat{\lambda} \cong 0.0138$ as the maximum likelihood estimator. The APPL statement

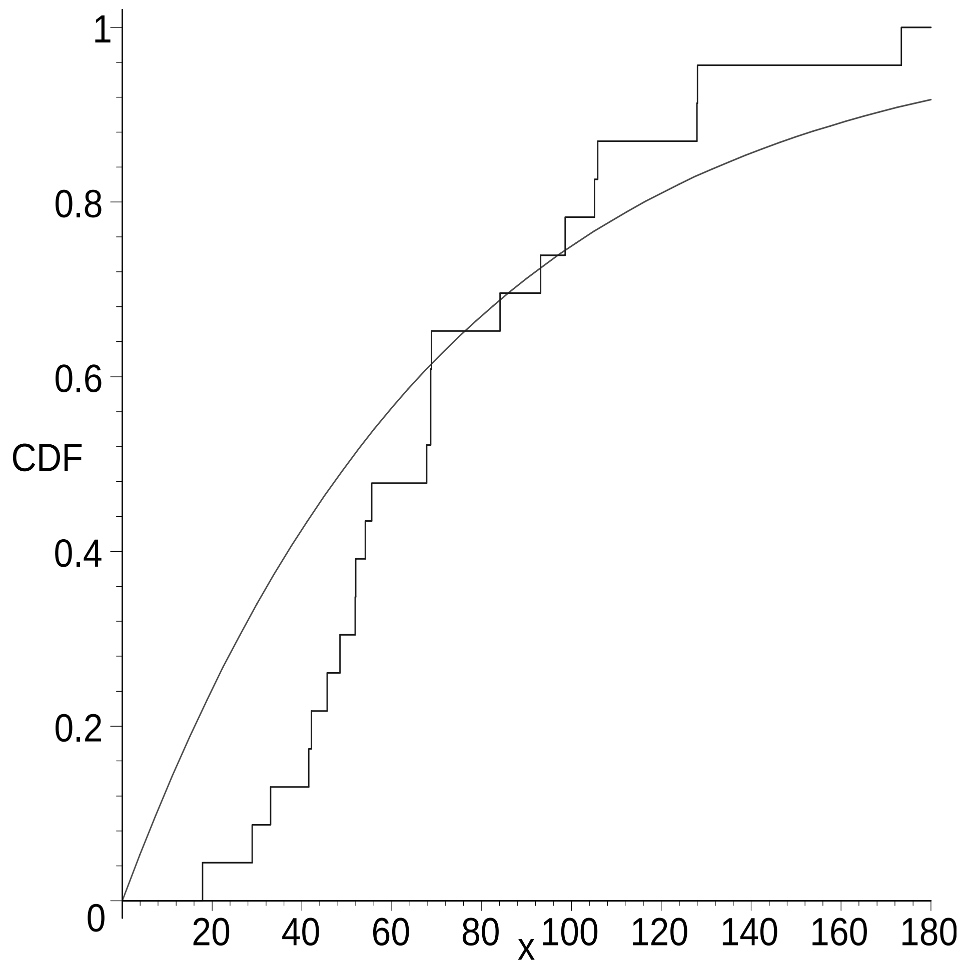
```
PlotEmpVsFittedCDF(X, BallBearing,
    [lambda = lamhat[1]], 0, 180);
```

produces a plot of the empirical and fitted CDFs.

To assess model adequacy, either a formal goodness-of-fit test can be performed, or goodness-of-fit statistics can be compared for competing models. The K–S test statistic is computed with the APPL statement

```
KSTest(X, BallBearing, [lambda = lamhat[1]]);
```

which returns 0.3068, indicating a rather poor fit.



Empirical and Fitted Exponential Cumulative Distribution
Functions for the Ball Bearing Data Set

Example 13. Fit the reciprocal of an exponential random variable to the service times in the previous example.

The distribution of the reciprocal of an exponential random variable is found with the statements

```
X := ExponentialRV(lambda);
g := [[x -> 1 / x], [0, infinity]];
Y := Transform(X, g);
```

which derives the PDF of Y to be

$$f_Y(y) = \frac{\lambda}{y^2} e^{-\lambda/y} \qquad\qquad y > 0$$

The MLE $\hat{\lambda} \cong 55.06$ is computed with the additional statement

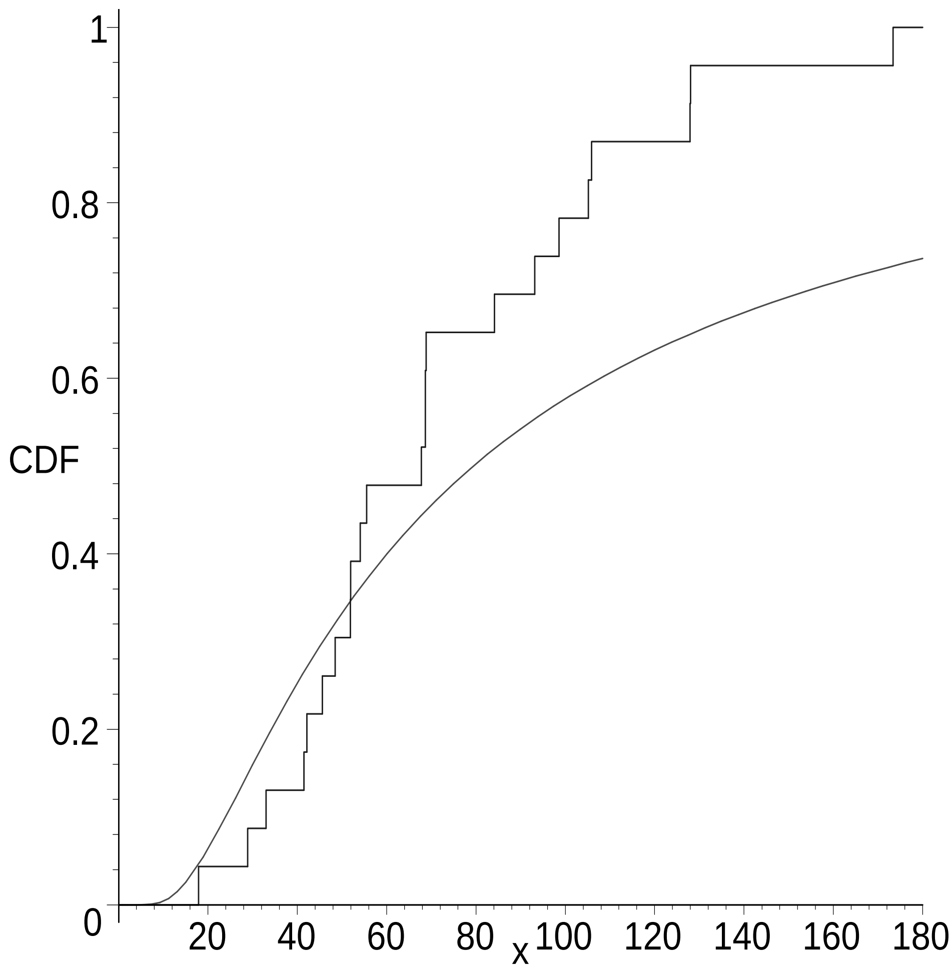
```
lamhat := MLE(Y, BallBearing, [lambda]);
```

Example 14. Fit the inverse Gaussian and Weibull distributions to the data set.
The statements

```
X := InverseGaussianRV(lambda, mu);
hat := MLE(X, BallBearing, [lambda, mu]);
KSValue := KSTest(X, BallBearing,
    [lambda = hat[1], mu = hat[2]]);
```

yield an improved fit with $\hat{\lambda} \cong 231.67$, $\hat{\mu} \cong 72.22$, and a K–S test statistic of 0.088.

The procedure `MLE` is able to return the appropriate values because the maximum likelihood estimators are in closed form for the inverse Gaussian distribution.



Empirical and Reciprocal Exponential Fitted Cumulative
Distribution Functions for the Ball Bearing Data Set

Example 14 continued. For the Weibull distribution, the statements

```
Y := WeibullRV(lambda, kappa);
hat := MLE(Y, BallBearing, [lambda, kappa]);
```

fail to return the MLEs. The Maple numerical equation solving procedure `fsolve` cannot exploit the structure in the score vector. `MLEWeibull` has been written to compute MLEs for the Weibull distribution.

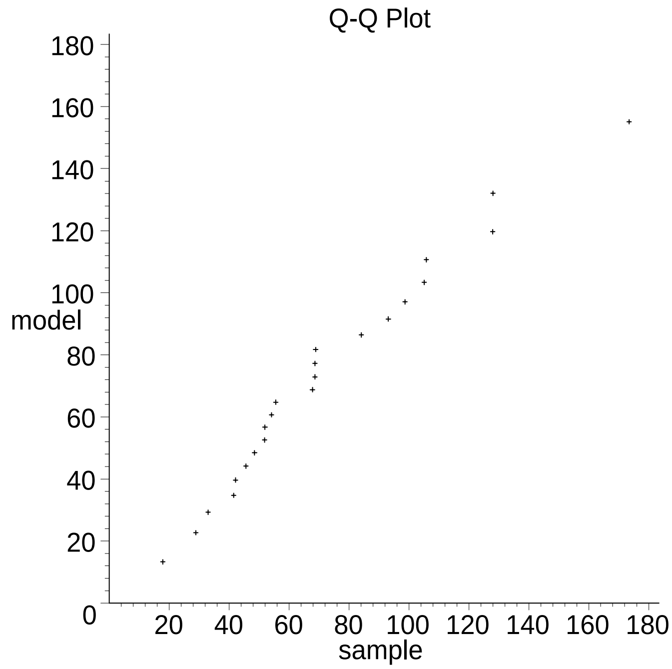
Fit can be assessed visually using a Q–Q or P–P plot (Law and Kelton, 2000, pages 352–358). The APPL statements

```
QQPlot(Y, BallBearing,
    [lambda = hat[1], kappa = hat[2]]);
PPPlot(Y, BallBearing,
    [lambda = hat[1], kappa = hat[2]]);
```

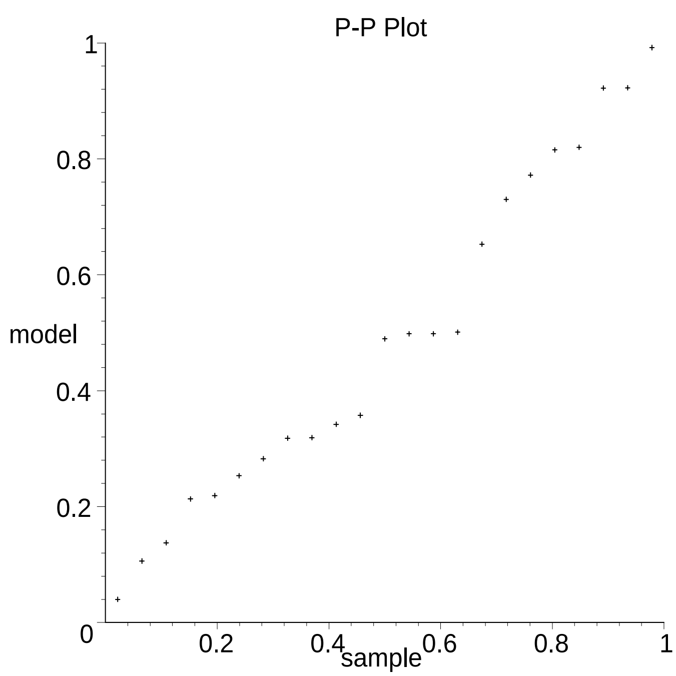
produce the plots for the Weibull distribution.

The K–S test statistic values for various distributions that were fit to the ball bearing data (in APPL) via maximum likelihood estimation

Model	Test statistic
Exponential	0.307
Reciprocal of Exponential	0.306
Weibull	0.151
Gamma	0.123
Arctangent	0.094
Log normal	0.090
Inverse Gaussian	0.088



Q–Q Plot of Ball Bearing Data with Fitted Weibull Distribution



P–P Plot of Ball Bearing Data with Fitted Weibull Distribution

Example 15. Determine an input model for the remission time for the treatment group in the study concerning the drug 6-MP (Gehan, 1965). An asterisk denotes a censored observation. The remission times (in weeks) are

6 6 6 6* 7 9* 10 10* 11* 13 16
17* 19* 20* 22 23 25* 32* 32* 34* 35*.

`MP6` and `MP6Censor` are pre-defined in APPL. `MP6` is simply the 21 data values given above, and `MP6Censor` is the list

```
[1, 1, 1, 0, 1, 0, 1, 0, 0, 1, 1,
   0, 0, 0, 1, 1, 0, 0, 0, 0, 0]
```

where 0 represents a censored value and 1 represents an uncensored value.

The statements used to determine the MLE for an exponential distribution are

```
X := ExponentialRV(lambda);
hat := MLE(X, MP6, [lambda], MP6Censor);
```

which yield $\hat{\lambda} = \frac{9}{359}$

The statements used to determine the MLE for a Weibull distribution are

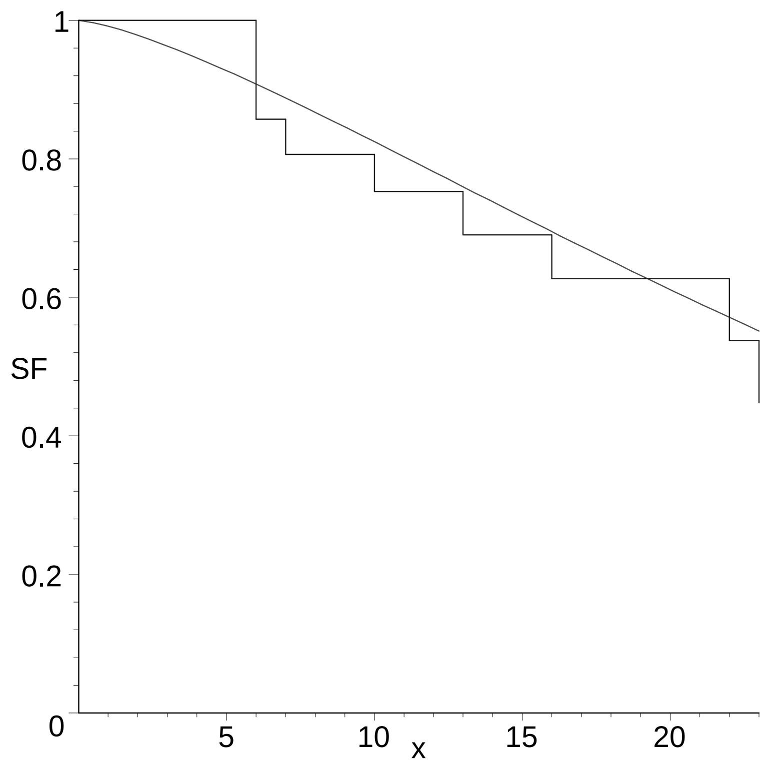
```
unassign('lambda');
unassign('kappa');
Y := WeibullRV(lambda, kappa);
hat := MLEWeibull(MP6, MP6Censor);
```

which yield $\hat{\lambda} \cong 0.03$ and $\hat{\kappa} \cong 1.35$

The Kaplan–Meier product-limit survivor function estimate for the **MP6** data set, along with the fitted Weibull survivor function are plotted using the APPL statement

```
PlotEmpVsFittedSF(Y, MP6,
    [lambda = hat[1], kappa = hat[2]],
    MP6Censor, 0, 23);
```

The downward steps in the estimated survivor function occur only at observed remission times.



Product–Limit Survivor Function Estimate and Fitted Weibull Survivor Function for the 6-MP Treatment Group

Example 16. A vending machine has capacity for 24 cans of "Purple Passion" grape drink. The machine is restocked to capacity every day at noon. Restocking time is negligible. The last five days have produced the following Purple Passion sales:

$$14 \qquad 24 \qquad 18 \qquad 20 \qquad 24.$$

The *demand* for Purple Passion at this particular vending machine can be estimated from the data by treating the 24-can sales figures as *right-censored* demand observations. If demand has the geometric distribution, with probability function

$$f(t) = p(1-p)^t \qquad t = 0, 1, 2, \ldots$$

find the MLE for $\hat{p}$.

Define a geometric random variable with the parameterization used above in a list of three sublists. The statements

```
X := [[x -> p * (1 - p) ^ x],
      [0 .. infinity],
      [`Discrete`, `PDF`]];
PurplePass := [14, 24, 18, 20, 24];
PurplePassCensor := [1, 0, 1, 1, 0];
MLE(X, PurplePass, [p], PurplePassCensor);
```

yield the MLE $\hat{p} = \frac{3}{103}$.

Example 17. Ignoring preventive maintenance, twelve odometer readings (from a certain model of car) associated with failures appearing over the first 100,000 miles are

12,942	28,489	65,561	78,254	83,639	85,603
88,143	91,809	92,360	94,078	98,231	99,900

Consider fitting a nonhomogeneous Poisson process to the above data set, where the ending time of the observation interval is assumed to be 100,000 miles. The data can be approximated by a power law process (i.e., the intensity function has the same parametric form as the hazard function for a Weibull random variable).

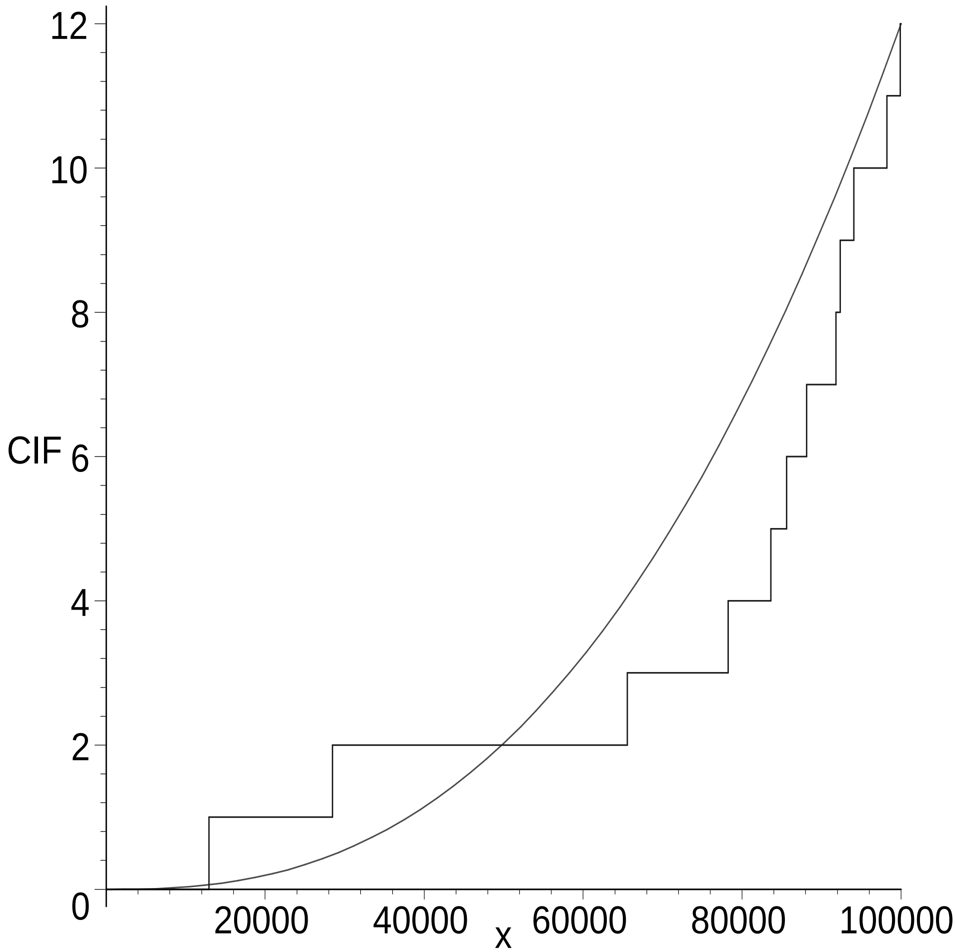
The following APPL statements return $\hat{\lambda} \cong 0.000026317$ and $\hat{\kappa} \cong 2.56800$:

```
CarFailures := [12942, 28489, 65561, 78254,
  83639, 85603, 88143, 91809, 92360, 94078,
  98231, 99900];
X := WeibullRV(lambda, kappa);
hat := MLENHPP(X, CarFailures,
                [lambda, kappa], 100000);
```

The statement

```
PlotEmpVsFittedCIF(X, Sample, [lambda = hat[1],
   kappa = hat[2]], 0, 100000);
```

produces a plot of the empirical cumulative intensity function and the Weibull cumulative hazard function.



Cumulative Intensity Function Estimate and Fitted Weibull Cumulative Hazard Function for the `CarFailures` data

Example 18. (Larsen and Marx, 2001, page 319) Hurricanes typically strike the eastern and southern coastal regions of the United States, although they occasionally sweep inland before completely dissipating. The U.S. Weather Bureau reported that during the period from 1900 to 1969 a total of 36 hurricanes moved as far as the Appalachian Mountains. The maximum 24-hour precipitation levels (measured in inches) recorded from those 36 storms during the time they were over the mountains are

31.00	2.82	3.98	4.02	9.50	4.50
11.40	10.71	6.31	4.95	5.64	5.51
13.40	9.72	6.47	10.16	4.21	11.60
4.75	6.85	6.25	3.42	11.80	0.80
3.69	3.10	22.22	7.43	5.00	4.58
4.46	8.00	3.73	3.50	6.20	0.67.

A histogram of the data suggests that the random variable X, which is the maximum 24-hour precipitation, might be well approximated by the gamma distribution.

The following statements find the method of moments estimates for the parameters λ and κ, where `Hurricane` is the above data set.

```
X := GammaRV(lambda, kappa);
hat := MOM(X, Hurricane, [lambda, kappa]);
```

The resulting estimates for the parameters are $\hat{\lambda} = \frac{954000}{4252153} \cong 0.224$ and $\hat{\kappa} = \frac{6952275}{4252153} \cong 1.64$

Further Work

- Most distributions containing 3 or 4 unknown parameters (e.g., the Johnson distributions) are not going to have closed-form maximum likelihood estimators
- Some distributions, such as the Erlang distribution, have both a discrete and a continuous parameter
- Some distributions have their unknown parameters as part of their support; e.g. $X \sim triangular(a, b, c)$
- Asymptotic confidence regions for unknown parameters based on the likelihood ratio statistic can be determined by plotting the appropriate contour of the log likelihood function

References

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