State-of-the-Art with Statistical Tolerance Regions: Methods and Applications, with Computing Demonstrations Using the R Package tolerance

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Before We Begin...

- ► You can download this presentation file and the corresponding R scripts from Derek Young's GitHub repo:
 - https://github.com/dsy109/Supplemental/tree/main/CSP%202022%20Trainings/tolerance
- ▶ If you plan to run the R examples concurrently, make sure you have the most recent versions installed for all of the packages listed at the top of the .R file
- ► This tutorial was developed and tested using R version 4.1.1





Outline of Topics

Purpose of Tutorial



Introduction

Normal Tolerance Intervals

Some Non-Normal Tolerance Intervals

Nonparametric Tolerance Intervals

Regression Tolerance Intervals

Multivariate Tolerance Regions

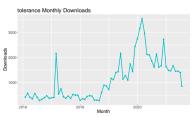
Final Comments





tolerance

- ► First release: 2009; see Young (2010) for technical details.
- The package includes: tolerance interval procedures for numerous parametric distributions, nonparametric settings, regression models, and some multivariate settings, as well as visualizations
- ▶ Used by NASA, 3M, EcoLab, PepsiCo, and NIST, among others
- ► The figure below also shows a mostly increasing trend over the years as the average number of monthly downloads per year is approximately 418, 592, 557, 1717, and 2203, in 2016, 2017, 2018, 2019, and 2020, respectively













Motivation: Tolerance Regions

- ► Based on a random sample, we have three primary statistical regions that can be calculated:
 - Confidence regions → provide regions for an unknown population parameter (e.g., mean vector, variance-covariance matrix)
 - ▶ Prediction regions → provide regions for one or more future observations from the sampled population
 - ► Tolerance regions → provide regions that are expected to contain at least a specified proportion of the sampled population
- ► Typical applications of tolerance regions (or **tolerance intervals** for the univariate setting) are found in clinical and industrial studies, statistical quality control, environmental monitoring, and setting statistically-based engineering design limits
- ► Used in regulations published by the Environmental Protection Agency (EPA), the Food and Drug Administration (FDA), the International Atomic Energy Agency (IAEA), and standard 16269-6 of the International Organization for Standardization (ISO)





Statistical Tolerance Sets

Definition

Let $\mathcal F$ be the class of all Borel measurable distributions in $\mathbb R^p$, $p\in\mathbb N$. Let $\mathcal X=\{\mathbf X_1,\dots,\mathbf X_n\}$ be an iid random sample of size n>p drawn from $F\in\mathcal F$, and $\mathbf X$ be a random vector that also follows F, independently of $\mathcal X$. Let $T(\mathcal X)$ be a random subset of $\mathbb R$ and define $C_F(T(\mathcal X))$ to be the probability content under F of the set $T(\mathcal X)$. If

$$\inf_{F \in \mathcal{F}} \Pr \left\{ C_F(T(\mathcal{X})) \ge P \right\} = 1 - \alpha,$$

then $T(\mathcal{X})$ is a $(1-\alpha, P)$ tolerance set, where $P, \alpha \in (0,1)$ are the (probability) content level and confidence level, respectively. If

$$E[C_F(T(\mathcal{X}))] = \beta,$$

then $T(\mathcal{X})$ is a β -expectation tolerance set, where $\beta \in (0,1)$ is the desired average content level of the tolerance set.

ightharpoonup β -expectation tolerance sets are just prediction sets





Normal Tolerance Intervals

Normal Tolerance Interval

- Introduction
- K-factors: [K.factor, K.table, K.factor.sim]
- Tolerance Limits for Normally Distributed Data: [normtol.int]
- Sample Size Determination: [norm.ss]
- Operating Characteristic (OC) Curves: [norm.OC]
- Application



Normal Tolerance Interval: Introduction

Suppose we have a random sample, X, from a normally distributed population. The one-sided tolerance interval is

$$(\bar{X} - k_1 s, \bar{X} + k_1 s)$$

The two-sided lower and upper tolerance interval is

$$(\bar{X} - k_2 s, \bar{X} + k_2 s)$$

respectively. Here, \bar{X} is the sample mean, s is the sample standard error, and k_1 and k_2 indicates k-factors for one-sides and two-sided tolerance intervals, respectively. Derivation of normal tolerance intervals depend on k-factors.





Methodology

There is a great deal of literature on normal tolerance intervals. tolerance package covers a range of these methods.

Before the wide availability of computers, approximation methods were deeply studied by various researchers, and approximation methods were developed and improved for different cases. Exact methods were later developed with the support of computer developments. tolerance covers exact methods and numerous approximations.



Methodology

EXACT:

One-Sided:

The k-factor ensures that we capture at least a proportion P of the sampled population with confidence level $(1-\alpha)$ is calculated as

$$k_1 = \frac{1}{\sqrt{n}} t_{n-1;1-\alpha}(\sqrt{n} Z_P)$$

where $t_{f;q}$ is the q^{th} quantile of a noncentral t-distribution with degree of freedom f and noncentrality parameter δ and z_q is the q^{th} quantile of the standard normal distribution.

Two-Sided:

There are no closed-form solutions for exact method for two-sided tolerance limits under normality, so one must use numerical methods.





Methodology

For a two-sided (P,γ) tolerance limits, the k-factor is the solution to The k-factor for two-sided (P,γ) tolerance limits are is

$$\sqrt{\frac{2n}{\pi}} \int_0^\infty P\left(\chi^2 n - 1 > \frac{(n-1)\chi_{1;P}^2(z^2)}{k_2(n,\alpha,P)^2}\right) e^{-\frac{1}{2}nz^2} dz = 1 - \alpha$$

Multiple approximation methods were proposed. (Note that approximation method can also be applied for one-sided tolerance limits.)

- weight Weissberg and Beatty (1960) used Newton's Method to approximate r and Cornish-Fisher approximation to estimated χ^2 distribution, based on (Wald & Wolfowitz, 1946).
- <u>HE2:</u> is a method based on Weissberg and Beatty (1960), but computationally simpler.
- **S** ELL: Ellison (1964) gives a correction of Weissberg-Beatty's method when f is not larger than N^2 .
- M: Krishnamoorthy and Mathew (2009) provide approximation solution to the exact method.
- 5 HE: is a method developed by Howe (1969) and is often viewed as being extremely accurate, even for small sample sizes.
- $\underline{\textbf{0}}$ Oven (1964)'s method gives more flexibility and is capable of controlling different tails while capturing a specified proportion P at a given confidence level $(1-\alpha)\times 100$.





Normal Tolerance Interval: k-factors

To find the k-factor of a (P, γ) tolerance tolerance interval for a given sample with size of n, we need to determine the following quantities:

- lacktriangle Sample size, n
- $oldsymbol{\circ}$ Content Level, P
- **3** Confidence Level, γ
- One-sided or Two-sided
- Method
- Obligation
 Degree of Freedom
- The maximum number of subintervals to be used for possible intergration





Normal Tolerance Interval: k-factors

We have three functions for a quick reference of k-factors.

- **1** K.factor: k-factor for a certain condition
- K.table: k-factors for multiple conditions
- $oldsymbol{\$}$ K.factor.sim: Estimating k-factors for simultaneous tolerance intervals based on normality



Normal Tolerance Interval: K.factor

```
K.factor(n, P, alpha, side=c(1,2), method= c("HE", "HE2", "WBE",
"ELL", "KM", "EXACT", "OCT"), f, m)
```

Description:

The k-factor is a critical component for a tolerance interval and it plays the role of 'z-score' in a confidence intervals and determines the width of a tolerance interval. K.factor estimates the k-factors for tolerance intervals based on normality.





Normal Tolerance Interval: K.factor

Examples: by method

- K.factor(n = 10, P = 0.95, side = 2, method = "HE")
- ❷ K.factor(n = 10, P = 0.95, side = 2, method = "WBE")
- K.factor(n = 10, P = 0.95, side = 2, method = "EXACT", m = 50)
- K.factor(n = 100, P = 0.95, side = 2, method = "HE")
- **5** K.factor(n = 100, P = 0.95, side = 2, method = "WBE")





Normal Tolerance Interval: K.factor

```
> K.factor(10, P = 0.95, side = 2, method = "HE")
[1] 3.407495
> K.factor(10, P = 0.95, side = 2, method = "WBE")
[1] 3.379442
> K.factor(10, P = 0.95, side = 2, method = "EXACT", m = 50)
[1] 3.393429
> K.factor(100, P = 0.95, side = 2, method = "HE")
Γ1] 2.233895
> K.factor(100, P = 0.95, side = 2, method = "WBE")
[1] 2.232787
> K.factor(100, P = 0.95, side = 2, method = "EXACT", m = 50)
[1] 2.233882
```





Normal Tolerance Interval: K.table

```
K.table(n, P, alpha, side = c(1,2), method = c("HE", "HE2", "WBE", "ELL", "KM", "EXACT", "OCT"), by arg = c("n", "alpha", "P"), f, m)
```

Description:

K.table tabulates k-factors for tolerance intervals based on normality under different conditions. Users can specify the presentation of the table with respect to the order of sample size (n), content level (P), or confidence level (α) .





Normal Tolerance Interval: K.table

Examples:

Ordered by sample size:

```
K.table(n = seq(50, 60, 10), alpha = c(0.01, 0.05, 0.10), P = c(0.90, 0.95, 0.99), by arg = "n")
```

Ordered by content level:

```
K.table(n = seq(50, 60, 10), alpha = c(0.01, 0.05, 0.10), P = c(0.90, 0.95), by.arg = "P")
```

Ordered by confidence level:

```
K.table(n = seq(50, 60, 10), alpha = c(0.01, 0.05), P = c(0.90, 0.95, 0.99), by.arg = "alpha")
```





Normal Tolerance Interval: K.table, by 'n'

```
> K.table(n = seg(50, 60, 10), alpha = c(0.01, 0.05, 0.10),
         P = c(0.90, 0.95, 0.99), bv.arg = "n")
$'50'
         0.9 0.95 0.99
0.99 1.820800 2.268898 3.124607
0.95 1.645565 2.064993 2.862449
0.9 1.559468 1.965294 2.734892
$'60'
         0.9 0.95 0.99
0.99 1.764060 2.202345 3.038258
0.95 1.608913 2.022159 2.807055
0.9 1.532029 1.933272 2.693524
```





Normal Tolerance Interval: K.table, by 'P'

```
> K.table(n = seg(50, 70, 10), alpha = c(0.01, 0.05, 0.10),
          P = c(0.90, 0.95), by.arg = "P")
$'0.9'
           50
                    60
                             70
0.99 1.820800 1.764060 1.721577
0.95 1.645565 1.608913 1.581218
0.9 1.559468 1.532029 1.511212
$'0.95'
           50
                    60
                             70
0.99 2.268898 2.202345 2.152633
0.95 2.064993 2.022159 1.989865
0.9 1.965294 1.933272 1.909031
```





Normal Tolerance Interval: K.table, by ' α '

```
> K.table(n = seq(50, 70, 10), alpha = c(0.01, 0.05),
         P = c(0.90, 0.95, 0.99), by.arg = "alpha")
$'0.99'
       0.9 0.95 0.99
50 1.820800 2.268898 3.124607
60 1.764060 2.202345 3.038258
70 1.721577 2.152633 2.973920
$'0.95'
       0.9 0.95 0.99
50 1.645565 2.064993 2.862449
60 1.608913 2.022159 2.807055
70 1.581218 1.989865 2.765393
```





Normal Tolerance Interval: K.factor.sim

```
K.factor.sim(n, P, alpha, side = c(1,2), method = c("EXACT", "BONF"),
m, l=number of population)
```

Description:

K.factor.sim estimates k-factors for simultaneous tolerance intervals based on normality. Two adjustment methodologies are included in this function.





K.factor.sim: Methodology

- **<u>EXACT:</u>** Mee (1990) developed simultaneous tolerance limits for different groups. For larger combinations of n and l when side=2 and method="EXACT", the calculation can be slow.
- <u>BONF:</u> In Krishnamoorthy and Mathew (2009), a *Bonferroni* correction method is introduced. For larger sample sizes when side = "BONF", there may be some accuracy issues with the 1-sided calculation since it depends on the noncentral t-distribution. The code is primarily intended to be used for moderate values of the noncentrality parameter. It will not be highly accurate, especially in the tails, for large values.



Normal Tolerance Interval: K.kactor.sim

Examples:





Normal Tolerance Interval: k.factor.sim

```
> KM_table
                           5
n
    5.419 4.485 4.111 3.914 3.795
    3.358 3.137 3.045 2.998 2.972
    2.800 2.705 2.668 2.652 2.646
    2.525 2.475 2.460 2.456 2.457
     2,356 2,329 2,323 2,325 2,329
  30 1.668 1.681 1.691 1.700 1.708
  40 1.611 1.623 1.633 1.641 1.648
  50 1.573 1.585 1.594 1.601 1.608
  60 1.546 1.557 1.565 1.572 1.579
  70 1.525 1.535 1.543 1.550 1.556
```





```
normtol.int(x, alpha, P, side = c(1,2), method = c("HE", "HE2",
"WBE", "ELL", "KM", "EXACT", "OCT"), m, log.norm = c(FALSE,TRUE))
```

Description:

normtol.int provides 1-sided or 2-sided tolerance intervals for data distributed according to either a normal distribution or log-normal distribution.

Derivation of normal-based tolerance intervals depends on the selection of k-factors, and therefore, 7 methods are included.





Examples:

- One-Sided:
 - normtol.int(x = x, alpha = 0.05, P = 0.95, side = 1,method =
 "HE", log.norm = FALSE)
- 2 Two-Sided:

```
normtol.int(x = x, alpha = 0.05, P = 0.95, side = 2, method = "HE", log.norm = FALSE)
```





```
set.seed(100)
x \leftarrow rnorm(100, 0, 0.2)
out1 <- normtol.int(x = x, alpha = 0.05, P = 0.95, side = 1,
                method = "HE", log.norm = FALSE)
out2 <- normtol.int(x = x, alpha = 0.05, P = 0.95, side = 2,
               method = "HE", log.norm = FALSE)
> out1
 alpha P x.bar 1-sided.lower 1-sided.upper
1 0.05 0.95 0.0005825125 -0.3927051
                                   0.3938701
> out2
 alpha P x.bar 2-sided.lower 2-sided.upper
1 0.05 0.95 0.0005825125 -0.4554493 0.4566144
```





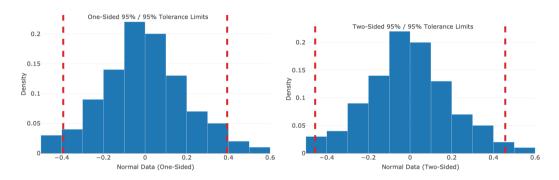


Figure: One-Sided v.s. Two-Sided



Sample Size Determination: norm.ss

```
norm.ss(x, alpha, P, side = 1, method = c("DIR", "FW", "YGZO"), m =
50, delta = NULL, P.prime = NULL, spec = c(NA, NA), hyper.par =
list(mu.0 = NULL, sig2.0 = NULL, m.0 = NULL, n.0 = NULL))
```

Description:

norm.ss provides minimum sample sizes for a future sample when constructing normal tolerance intervals. Various strategies are available for determining the sample size, including strategies that incorporate known specification limits.





norm.ss Methodology

Methodology:

- <u>DIR</u>: is the direct method (intended as a simple calculation for planning purposes) where the mean and standard deviation are taken as truth and the sample size is determined with respect to the given specification limits.
- <u>FW:</u> is for the traditional Faulkenberry-Weeks approach for sample size determination (Faulkenberry & Weeks, 1968).
- YGZO: is for the Young-Gordon-Zhu-Olin approach, which incorporates historical data and specification limits for determining the value of delta and/or P.prime in the Faulkenberry-Weeks approach (Young, Gordon, Zhu, & Olin, 2016).





Sample Size Determination: norm.ss

Examples:

Direct Method:

```
norm.ss(alpha = 0.05, P = 0.95, side = 2, spec = c(-3, 3), method = "DIR", hyper.par = list(mu.0 = 0, sig2.0 = 1))
```

FW Method:

```
norm.ss(alpha = 0.05 , P = 0.90, delta = 0.10 , P.prime = 0.97 , side = 2 , m = 50 , method = "FW")
```

YGZO Method:

```
norm.ss(x = rnorm(100 , mean = 0, sd = 3) , alpha = 0.05 , P = 0.90, delta = 0.10 , side = 2 , m = 50 , method = "YGZO" , spec = c(-2, 2), hyper.par = list(mu.0 = 0, sig2.0 = 1))
```





Sample Size Determination: norm.ss

```
> set_seed(100)
### DTR Method ###
> norm.ss(alpha = 0.05, P = 0.95, side = 2, spec = c(-3, 3),
         method = "DIR", hyper.par = list(mu.0 = 0, sig2.0 = 1))
alpha P delta P.prime
        0.05 0.95
### FW Method ###
> norm.ss(alpha = 0.05 , P = 0.90, delta = 0.10 , P.prime = 0.97 ,
         side = 2 , m = 50 , method = "FW")
 alpha P delta P.prime n
1 0.05 0.9 0.1
                   0.97 60
### YGZO Method ###
> norm.ss(x = rnorm(100 , mean = 0, sd = 3) , alpha = 0.05 , P = 0.90, delta = 0.10 ,
         side = 2 . m = 50 . method = "YGZO" . spec = c(-2, 2).
         hyper.par = list(mu.0 = 0, sig2.0 = 1))
alpha P delta P.prime n
1 0 05 0 9 0 1 0 9544997 117
```





```
norm.OC(alpha, P, n, side = c(1,2), method = c("HE", "HE2", "WBE", "ELL", "KM", "EXACT", "OCT"), k, m)
```

Description:

norm.OC provides OC-type curves to illustrate how values of the k-factors for normal tolerance intervals, confidence levels, and content levels change as a function of the sample size.





Examples:

By content level:

```
norm.OC(k = 4, alpha = NULL, P = c(0.90, 0.95, 0.99), n = 10:20, side = 1)
```

By confidence level:

```
norm.OC(k = 4, alpha = c(0.01, 0.05, 0.10), P = NULL, n = 10:20, side = 1)
```

By sample size:

```
norm.OC(k = NULL, P = c(0.90, 0.95, 0.99),
alpha=c(0.01,0.05,0.10), n = 10:20, side = 1)
```





```
plotly.norm.OC(k = 4, alpha = NULL, P = c(0.90, 0.95, 0.99),
             n = 10:20, side = 1.
             x.cex = 8. line.width = 4.
             v.lab.size = 16, x.lab.size = 16.
             x.tick.size = 16, v.tick.size = 16.
             title.size = 16, legend.size = 12)
plotlv.norm.OC(k = 4. alpha = c(0.01, 0.05, 0.10), P = NULL.
             n = 10:20, side = 1.
             x.cex = 8, line.width = 4,
             v.lab.size = 16, x.lab.size = 16,
             x.tick.size = 16, v.tick.size = 16,
             title.size = 16, legend.size = 12)
plotly.norm.OC(k = NULL, P = c(0.90, 0.95, 0.99).
             alpha=c(0.01,0.05,0.10), n = 10:20, side = 1,
             x.cex = 8, line.width = 4.
             v.lab.size = 16. x.lab.size = 16.
             x.tick.size = 16, v.tick.size = 16,
             title.size = 16, legend.size = 12)
```





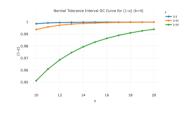


Figure: By P

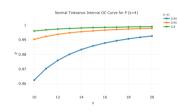


Figure: By $(1-\alpha)$

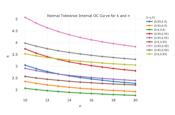


Figure: By n





Normal Tolerance Interval: Application

Normal distribution is not always seen in practice. For example, a mass production process usually requires quality control process and certain measurements might only follow a normal distribution approximately.

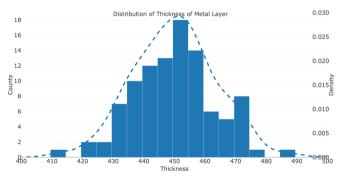
One illustrative example is the thickness of a metal layer on n=100 silicon wafers resulting from a chemical vapor deposition (CVD) process in a semiconductor plant; see Example 3.2 of Montgomery (2020).



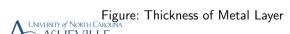


Application: Data

This distribution of the thickness of a metal layer on 100 silicon wafers resulting from a chemical vapor deposition (CVD) process in a semiconductor plant is shown in Figure 5.







Application: Tolerance Limits

The two-sided $(P,\gamma)=(0.95,0.95)$ tolerance limits for thickness data are (420.015~,~480.005) and are presented in Figure 6.

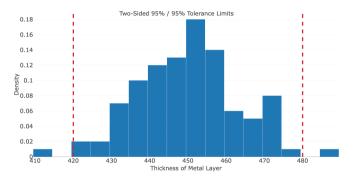


Figure: Two-Sided Tolerance Limits





Some Non-Normal Tolerance Intervals

Some Non-normal Tolerance Intervals

- Introduction
- ② Discrete Type
 - Example: Tolerance Limits for Binomial Distribution [bintol.int]
 - Example: Tolerance Limits for Poisson Distribution [poistol.int]
- Continuous Type
 - Example: Tolerance Limits for Weibull Distribution [exttol.int]
 - Example: Tolerance Limits for Gamma Distribution [gamtol.int]
- Application





Non-normal Tolerance Interval: Introduction

Although normality is the most commonly seen condition under many situations, non-normal distributions are perhaps just as frequently encountered. The tolerance package also handles common non-normal distributions. We illustrate the functionalities of tolerance package by presenting four classical non-normal distributions. More specifically, tolerance intervals for binomial, Poisson, Weibull and gamma distributions are presented.





```
bintol.int(x, n, m = NULL, alpha = 0.05, P = 0.99, side = 1, method =
c("LS", "WS", "AC", "JF", "CP", "AS", "LO", "PR", "PO", "CL", "CC",
"CWS"), a1 = 0.5, a2 = 0.5)
```

Description:

bintol.int Provides 1-sided or 2-sided tolerance intervals for binomial random variables. From a statistical quality control perspective, these limits use the proportion of defective (or acceptable) items in a sample to bound the number of defective (or acceptable) items in future productions of a specified quantity.

- \bullet <u>x:</u> Number of defective (or acceptable) units.
- ② <u>n:</u> Current lot size. $(\hat{p} = \frac{x}{n})$
- 3 m: Future lot size.





Methodology

Interval calculation for a *Binomial* distribution is complex and numerous methods are developed. (For more details, please see Brown, Cai, and DasGupta (2001)). bintol.int equips multiple methods:

- "LS": The large-sample method (the default method), which is appropriate when the sample size is large (e.g., $n \geq 50$) and $n\hat{p}$ and $n(1-\hat{p})$ are both ≥ 10 . Otherwise, the coverage may not achieve the nominal level.
- <u>"WS":</u> Wilson's method, which is appropriate even when the sample size is small (e.g., $n \le 40$). The coverage probability fluctuates acceptably near the nominal level provided p does not approach 0 or 1.
- "AC": The Agresti-Coull method, which is appropriate when the sample size is large (e.g., $n \ge 40$). This method is comparable to Wilson's method for large n.





Methodology

- "JF": Jeffreys' method, which is a Bayesian approach to the estimation. For this method, the prior distribution for p is assumed to be a beta distribution with parameters a1 and a2, both of which must be specified by the user.
- ② "CP": The Clopper-Pearson method (sometimes referred to as an "exact" procedure due to its derivation from the binomial distribution), which provides a more conservative interval and can be much larger than the nominal level as $n \to \infty$.
- $^{\bullet}$ <u>"AS":</u> The arcsine method, which is appropriate when p is not too close to 0 or 1. Otherwise, the coverage approaches 0.
- <u>"L0":</u> The logit method, which is appropriate when p is not too close to 0 or 1, but yields a more conservative interval.





Examples:

- Tolerance Limits using Multiple Methods:
 - ▶ bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15, P = 0.90, side = 2, method = "LS")
 - ▶ bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15, P = 0.90, side = 2, method = "AS")
- Tolerance Limits using Jeffreys' Methods:
 - ▶ bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15, P = 0.90, side = 1, method = "JF", a1 = 2, a2 = 10)
 - ▶ bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15, P = 0.90, side = 1, method = "JF", a1 = 5, a2 = 1)





```
> bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15, P = 0.90,
          side = 2. method = "LS")
  alpha P p.hat 2-sided.lower 2-sided.upper
1 0.15 0.9 0.23
                          494
> bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15. P = 0.90.
            side = 2, method = "AS")
  alpha P p.hat 2-sided.lower 2-sided.upper
1 0.15 0.9 0.23
                           495
> bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15, P = 0.90,
            side = 1, method = "JF", a1 = 2, a2 = 10)
 alpha P p.hat 1-sided.lower 1-sided.upper
1 0 15 0 9 0 23
                           513
> bintol.int(x = 230, n = 1000, m = 2500, alpha = 0.15, P = 0.90,
            side = 1. method = "JF", a1 = 5, a2 = 1)
 alpha P p.hat 1-sided.lower 1-sided.upper
1 0.15 0.9 0.23 523
```





```
poistol.int(x, n, m = NULL, alpha = 0.05, P = 0.99, side = 1, method
= c("TAB", "LS", "SC", "CC", "VS", "RVS", "FT", "CSC"))
```

Description:

poistol.int Provides 1-sided or 2-sided tolerance intervals for Poisson random variables. From a statistical quality control perspective, these limits bound the number of occurrences (which follow a Poisson distribution) in a specified future time period.

- **1** $\underline{\mathbf{x}}$: The number of occurrences of the event in time period n.
- ② $\underline{\mathbf{n}}$: The time period of the original measurements. $(\hat{\lambda} = \frac{x}{n})$
- <u>m:</u> Future time period.





Methodology

tolerance package includes seven methods calculating tolerance intervals with an underlying *Poisson* distribution. Two methods, tabulation and large-sample methods, build the foundation while others provide continuity and variance stabilization corrections.

- TAB: tabular method and is usually preferred for a smaller number of occurrences. This is the default method.
- 2 LS: the large-sample (Wald) method, which is usually preferred when the number of occurrences is x>20.
- 3 CC: gives a continuity-corrected version of the large-sample method.
- <u>VS:</u> gives a variance-stabilized version of the large-sample method.
- <u>RVS:</u> is a recentered version of the variance-stabilization method.
- SC: the score method, which again is usually used when the number of occurrences is relatively large.
- <u>CSC:</u> is the continuity-corrected version of the score method.
- 8 FT: is the Freeman-Tukey method.





Methodology

Tabular Method

Hahn and Meeker (2011) shows that one-sided limits has the form

$$\lambda_L = \frac{\chi_{2x;\alpha}^2}{2n}$$

$$\lambda_U = \frac{\chi_{2x+2;1-\alpha}^2}{2n}$$

where n is the sample size and $\chi^2_{d;1-\alpha}$ is the $(1-\alpha)^{th}$ quantile of a χ^2 distribution with d degrees of freedom.



Large-Sample Method

Hahn and Meeker (2011) also utilized large-sample theory and that one-sided limits has the form

$$\lambda_L = \hat{\lambda} - z_{1-\alpha} \sqrt{\frac{\hat{\lambda}}{n}}$$

$$\lambda_U = \hat{\lambda} + z_{1-\alpha} \sqrt{\frac{\hat{\lambda}}{n}}$$

- This method performs quite good and usually is preferred for n > 20.
- For both methods in two-sided setting, simply replace α by $\frac{\alpha}{2}$ and P by $\frac{P+1}{2}$. Further details on *Poisson* tolerance intervals can be found in Hahn and Chandra





Examples:

One-sided:

- poistol.int(x = 45, n = 9, m = 3, alpha = 0.05, P = 0.90, side = 1,
 method = "TAB")
- ▶ poistol.int(x = 45, n = 9, m = 3, alpha = 0.05, P = 0.90, side = 1, method = "LS")

Two-sided:

- ▶ poistol.int(x = 45, n = 9, m = 15, alpha = 0.05, P = 0.90, side = 2, method = "TAB")
- ▶ poistol.int(x = 45, n = 9, m = 15, alpha = 0.05, P = 0.90, side =
 2, method = "LS")





```
### One-Sided ###
> poistol.int(x = 45, n = 9, m = 3, alpha = 0.05, P = 0.90,
           side = 1. method = "TAB")
 alpha P lambda.hat 1-sided.lower 1-sided.upper
1 0.05 0.9
> poistol.int(x = 45, n = 9, m = 3, alpha = 0.05, P = 0.90,
           side = 1, method = "LS")
 alpha P lambda.hat 1-sided.lower 1-sided.upper
1 0 05 0 9
### Two-Sided ###
> poistol.int(x = 45, n = 9, m = 15, alpha = 0.05, P = 0.90,
           side = 2. method = "TAB")
 alpha P lambda.hat 2-sided.lower 2-sided.upper
1 0.05 0.9
> poistol.int(x = 45, n = 9, m = 15, alpha = 0.05, P = 0.90,
           side = 2. method = "LS")
 alpha Plambda.hat 2-sided.lower 2-sided.upper
1 0.05 0.9 5
                                    113
```





```
exttol.int(x, alpha = 0.05, P = 0.99, side = 1, dist = c("Weibull", "Gumbel"), ext = c("min", "max"), NR.delta = 1e-8)
```

Description:

exttol.int Provides 1-sided or 2-sided tolerance intervals for data distributed according to either a Weibull distribution or extreme-value (also called Gumbel) distributions.

- ext: If dist = "Gumbel", then select which extreme is to be modeled for the Gumbel distribution. The Gumbel distribution for the minimum (i.e., ext = "min") corresponds to a left-skewed distribution and the Gumbel distribution for the maximum (i.e., ext = "max") corresponds to a right-skewed distribution.
- NR.delta: The stopping criterion used for the Newton-Raphson algorithm when finding the maximum likelihood estimates of the Weibull or extreme-value distribution.





Methodology

Weibull and Gumbel distributions are two representative distribution measuring extreme events. They have wide applications in the fields such as physics and engineering. tolerance package supplies tolerance interval calculations for both distribution.

A random variable X has a Weibull distribution has a cumulative distribution function

$$F_X(x;\theta,\beta) = 1 - e^{-(\frac{x}{\theta})^{\beta}}$$

where x>0 with shape parameter $\beta>0$ and scale parameter $\theta>0$. Let a random variable Y=ln(X), then Y follows a extreme-value distribution (also called *Gumbel* distribution for the minimum), and it has the cumulative distribution

$$F_Y(y;\xi,\delta) = 1 - e^{-e^{\frac{y-\xi}{\delta}}}$$

A random variable Z is said to have a Gumbel distribution for the maximum if it has the cumulative density function of

$$F_Y(y;\xi,\delta) = 1 - e^{-e^{-\frac{y-\xi}{\delta}}}$$

where $-\infty < y < +\infty, -\infty < \xi = ln(\theta) < +\infty$, and $\delta = \frac{1}{\beta} > 0$. Newton-Raphson algorithm is used to estimate parameters for *Gumbel* distributions.





According to Bain and Engelhardt (1981), the formula for estimating the 1-sided extreme-value tolerance limits are

$$L = \hat{\xi} - \frac{\delta t_{n-1;\alpha}^*(-\sqrt{n}\lambda_P)}{\sqrt{n-1}}$$

$$U = \hat{\xi} - \frac{\hat{\delta} t_{n-1;1-\alpha}^*(-\sqrt{n}\lambda_{1-P})}{\sqrt{n-1}}$$

Furthermore, the formulas for estimating the 1-sided Weibull tolerance limits are

$$L_W = e^L$$

$$U_W = e^U$$





For a *Gumbel* distribution for a maximum, the maximum likelihood estimates of the parameter $(\hat{\xi} \text{ and } \hat{\delta})$ can be found by using a Newton-Raphson algorithm. The formula for estimating the one-sided tolerance limits for the *Gumbel* distribution for the maximum are

$$L = \hat{\xi} + \frac{\delta t_{n-1;\alpha}^*(-\sqrt{n}\lambda_{1-P})}{\sqrt{n-1}}$$

$$U = \hat{\xi} + \frac{\hat{\delta} t_{n-1;1-\alpha}^*(-\sqrt{n}\lambda_P)}{\sqrt{n-1}}$$





Examples:

exttol.int provides tolerance interval calculations for both *Weibull* and *Gumbel* distributions. When *Gumbel* distribution is selected, the *Gumbel* distribution for the minimum or maximum need to be further specified.

- Weibull Distribution:
 - exttol.int(x = x, alpha = 0.15, P = 0.90, side = 1, dist = "Weibull")
- @ Gumbel Distribution:

```
exttol.int(x = GumbelData, alpha = 0.15, P = 0.90, side = 2, dist
= "Gumbel" , ext = "max")
```





```
## 85%/90% 1-sided Weibull tolerance intervals for a sample
## of size 150.
> set.seed(100)
> WeibullData <- rweibull(150, 3, 75)
> out <- exttol.int(x = WeibullData, alpha = 0.15, P = 0.90, side = 1,
                 dist = "Weibull")
> out.
 alpha P shape.1 shape.2 1-sided.lower 1-sided.upper
1 0.15 0.9 3.084836 74.48706
                               33.87539
                                            101.0331
## 85%/90% 2-sided Gumbel distribution for the maximum tolerance intervals
## for a sample of size 200.
> set.seed(100)
> GumbelData <- rgumbel(200, loc=3, scale=5)</pre>
> out <- exttol.int(x = GumbelData, alpha = 0.15, P = 0.90, side = 2,
                  dist = "Gumbel" , ext = "max")
> 0111
 alpha P shape.1 shape.2 2-sided.lower 2-sided.upper
1 0.15 0.9 3.504217 4.791701 -2.422067
                                            19.01293
```





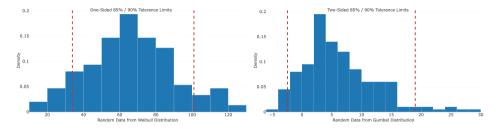


Figure: Tolerance Limits for Weibull and Gumbel Distributions





```
gamtol.int(x, alpha = 0.05, P = 0.99, side = 1, method = c("HE",
"HE2", "WBE", "ELL", "KM", "EXACT", "OCT"), m = 50, log.gamma =
FALSE)
```

Description:

gamtol.int Provides 1-sided or 2-sided tolerance intervals for data distributed according to either a gamma distribution or log-gamma distribution.

- \bullet method: method here is specified for computing the k-factor for normal tolerance limits.
- ② <u>m:</u> The maximum number of subintervals to be used in the integrate function. This is necessary only for method = "EXACT" and method = "OCT". The larger the number, the more accurate the solution, with the trade-off of slowing the calculation.





Methodology

Krishnamoorthy, Mathew, and Mukherjee (2008) developed the tolerance limits for a *Gamma* distribution based on a normal approximation.

A random variable X is $\operatorname{\textit{gamma}}$ distributed if it has the cumulative distribution function

$$F_X(x;\theta,\beta) = \int_{t=0}^x \frac{t^{\theta-1}e^{-\frac{t}{\beta}}}{\beta^{\theta}\Gamma(\theta)}dt$$

where $x>0,\ \theta>0$ is a shape parameter and $\beta>0$ is a scale parameter, and $\Gamma(\cdot)$ is the gamma function.

If X follows a Gamma distribution, the $X^{\frac{1}{3}}$ is approximately a normal distribution with mean μ and variance σ^2 such that

$$\mu = \frac{\beta^{\frac{1}{3}}\Gamma(\theta + \frac{1}{3})}{\Gamma(\theta)} \quad ; \quad \sigma^2 = \frac{\beta^{\frac{2}{3}}\Gamma(\theta + \frac{2}{3})}{\Gamma(\theta)} - \mu^2$$





Since $X^{\frac{1}{3}}$ follows a normal distribution approximately, corresponding tolerance limits can be found in the setting for *Normal* distribution such that

$$(L_N, U_N) = \hat{\mu} \pm k\hat{\sigma}$$

(Note: method argument in gamtol.int is used here.)

Once the above limits are calculated, they need to be transferred back to obtain tolerance limits for a *Gamma* distribution such that

$$(L,U) = (L_N^3, U_N^3)$$

If X^* is a log-gamma random variable, then $ln(X^* = X \text{ follows a } \textit{Gamma} \text{ distribution})$. Then an extra step needs to be done to obtain the tolerance limits for X^* such that

$$(L^*, U^*) = (e^L, e^U)$$





Examples:

One-Sided:

```
gamtol.int(x = x, alpha = 0.01, P = 0.99, side = 1, method = "HE")
```

Two-Sided:

```
gamtol.int(x = x, alpha = 0.05, P = 0.95, side = 2, method = "EXACT")
```



```
> set.seed(100)
> x < - rgamma(50, 0.30, scale = 2)
## 99%/99% 1-sided gamma tolerance intervals for a sample
## of size 50, using Howe method.
> out1 <- gamtol.int(x = x, alpha = 0.01, P = 0.99, side = 1,
                   method = "HE")
> out.1
  alpha P 1-sided.lower 1-sided.upper
1 0.01 0.99
                                6.769559
## 95%/95% 2-sided gamma tolerance intervals for a sample
## of size 50, using EXACT method.
> out2 <- gamtol.int(x = x, alpha = 0.05, P = 0.95, side = 2,
                     method = "EXACT")
> 011±2
  alpha P 2-sided.lower 2-sided.upper
1 0.05 0.95
                                3.983218
```





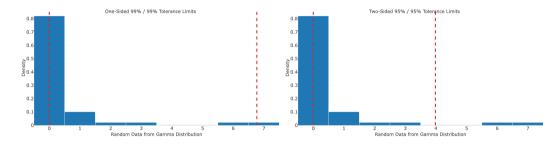


Figure: Tolerance Limits Gamma Distributions





Application: Binomial Distribution

A proportion control chart is a representative illustration of a *Binomial* distribution since products will be categorized as either good or defective.

30 wafers of chips were selected for quality control process. On each wafer 50 chips are measured and a defective is defined whenever a misregistration, in terms of horizontal and/or vertical distances from the center, is recorded. Numerical data can be found here.

Suppose we want to calculate the tolerance limits for a future wafer of 50 chips. bintol.int can be therefore applied. In addition, plotly.plot.control returns the corresponding control chart.

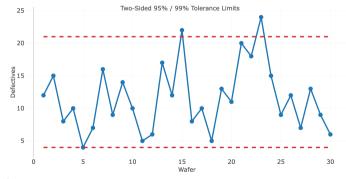
```
> binom.app <- bintol.int(x=defects, n=50*30,
m=50, alpha=0.05, P=0.99, side=2, method="CP")
> binom.app
alpha P p.hat 2-sided.lower 2-sided.upper
1 0.05 0.99 0.2313333 4 21
```





Application: Binomial Distribution

defects contains data of number of defectives for 30 wafers, n is total number of chips and m is the future lot size, which is one wafer (50) of chips. The two-sided $(P,\gamma)=(0.99,0.95)$ tolerance limits is (4,21).







Application: Poisson Distribution

As is well known that a *Poisson* distribution returns the probability of number of occurrence of an event within a certain period of time. Doctors visits is a great example to demonstrate a *Poisson* distribution.

Cameron and Trivedi (1986) provided doctors visits data which include 5190 patients' data of doctors visits over the span of 2 weeks. Actual dataset is embedded in AER package.

Suppose we are interested in the tolerance limits of number of visits for the next 10 individuals. *poistol.int* shall be applied to compute the tolerance limits for a *Poisson* distribution.

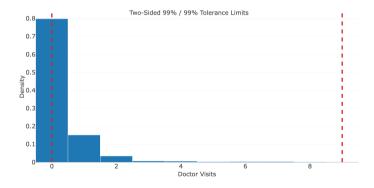
```
> library(AER)
> data("DoctorVisits")
> visits <- DoctorVisits$visits
> pois.app <- poistol.int(x=visits, n=length(visits), m=10,
alpha=0.01, P=0.99, side=2, method="TAB")
> pois.app
alpha P lambda.hat 2-sided.lower 2-sided.upper
1 0.01 0.99 0.3017341 0 9
```





Application: Poisson Distribution

The two-sided $(P,\gamma)=(0.99,0.99)$ tolerance limits for this *Poisson* distributed is (0,9).







Application: Weibull Distribution

Harris and Boyd (1995) provided kidney function data of 596 participants with 5 different measurements.

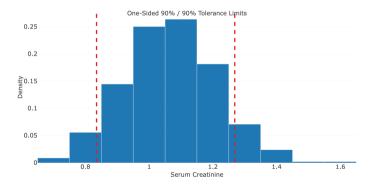
Suppose we are interested in the tolerance limits of serum creatinine of those 596 participants, *exttol.int* is a good option to compute the tolerance limits for a *Weibull* distribution.





Application: Weibull Distribution

The one-sided $(P, \gamma) = (0.90, 0.90)$ lower tolerance limits for this *Weibull* distributed data is 0.835 and upper tolerance limits is 1.269.







Application: Gamma Distribution

Lee and Wang (2003) provided a sample of remission time data for bladder cancer patients. The remission time follow a *Gamma* distribution approximately. Suppose we would like to calculate a one-sided upper tolerance limits for the sample data, *gamtol.int* shall be used in this case.

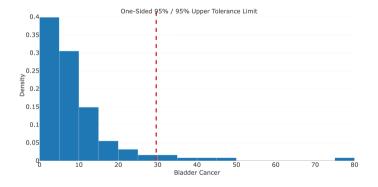
```
> bladder <- unlist(read.table("https://raw.githubusercontent.com/dsy109/Supplemental/main/
CSP%202022%20Trainings/tolerance/Datasets/bladder.txt",header=FALSE))
> gamma.app <- gamtol.int(x=bladder, alpha=0.05, P=0.95, side=1)
> gamma.app
alpha    P 1-sided.lower 1-sided.upper
1    0.05    0.95    0.3655981    29.64082
```





Application: Gamma Distribution

The one-sided $(P, \gamma) = (0.95, 0.95)$ upper tolerance limits for this *Gamma* distributed bladder data 29.641.







Nonparametric Tolerance Intervals

Nonparametric Tolerance Intervals

- Introduction
- Nonparametric Tolerance Intervals: [nptol.int]
- **3** β -Expectation Tolerance Interval: [npbetol.int]
- Sample Size Determination: [np.order]
- Application





Nonparametric Tolerance Interval: Introduction

Occasionally, a researcher may not wish to make any distributional assumption regarding their data. All that is assumed about the random sample $X_1=x_1,\cdots,X_n=x_n$ is that the underlying distribution function F_X is a continuous, non-decreasing, probability distribution.

The basic form of the (P,γ) nonparametric tolerance limits are

$$L = x_{[r]}$$
 ; $U = x_{[s]}$

where $x_{[j]}$ corresponds to the j^{th} order statistics of the sample data.





Methodology

Computing nonparametric tolerance intervals involves finding the appropriate r and s values ($x_{[r]}$ and $x_{[s]}$), which is typically done using the *Beta* or *Binomial* distribution.

- <u>"HM":</u> The Hahn-Meeker method (Hahn & Meeker, 2011), which uses an estimate based on the binomial distribution; however, two intervals may be reported if an odd number of observations must be trimmed from both sides.
- <u>"WILKS":</u> The Wilks method (Wilks, 1941), which uses an estimate based on the beta distribution to omit a certain number of observations from either side. For the two-sided intervals, the tolerance intervals are symmetric about the center of the observed data.
- <u>"WALD":</u> The Wald method (Wald, 1943), which is the same as the Wilks method for the one-sided setting. For the two-sided setting, symmetry about the center of the observed data is not assumed and this method finds all possible tolerance intervals, each having at least the specified confidence level.
- <u>"YM":</u> The the Young-Mathew method (Young & Mathew, 2014) for performing interpolation or extrapolation based on the order statistics.





```
nptol.int(x, alpha, P, side = c(1,2), method = c("WILKS", "WALD",
"HM", "YM"), upper, lower)
```

Description:

nptol.int provides 1-sided or 2-sided nonparametric (i.e., distribution-free) tolerance intervals for any continuous data set.

<u>Note</u>: we also add an important option for users to specify a certain upper or lower bound based on their professionalism.





Examples:

- One-Sided:
 - nptol.int(x = x, alpha = 0.10, P = 0.90, side = 1, method =
 "WILKS", upper = NULL, lower = NULL)
- Two-Sided (with a specified upper bound):
 nptol.int(x = x, alpha = 0.10, P = 0.90, side = 2, method =
 "WILKS", upper = NULL, lower = NULL)



```
set.seed(100)
x \leftarrow rlogis(100, 5, 1)
out1 <- nptol.int(x = x, alpha = 0.10, P = 0.90, side = 1,
              method = "WILKS", upper = NULL, lower = NULL)
out2 <- nptol.int(x = x, alpha = 0.10, P = 0.90, side = 2,
      method = "WILKS", upper = NULL, lower = NULL)
> 011±1
 alpha P 1-sided.lower 1-sided.upper
1 0.1 0.9 3.056274 7.563949
> out2
 alpha P 2-sided.lower 2-sided.upper
1 0.1 0.9
              2.18245 8.377662
```





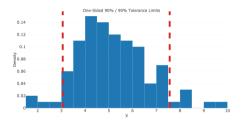


Figure: 1-Sided

```
plotly.plottol.hist(out1 , x=x , side = "two" , x.lab = "X", tol.lwd = 18 , x.lab.size = 36 , x.tick.size=36 , y.lab.size = 36 , y.tick.size = 36 , title.size = 36 , title.position.y = 0.995)

College of Arts and Sciences ASHEVILLE
```

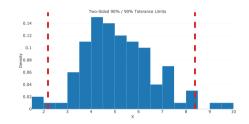


Figure: 2-Sided

```
npbetol.int(x, Beta, side = c(1,2), upper, lower)
```

Description:

npbetol.int provides 1-sided or 2-sided nonparametric (i.e., distribution-free) beta-expectation tolerance intervals for any continuous data set. These are equivalent to nonparametric prediction intervals based on order statistics.





Examples:

- ① One-Sided:
 npbetol.int(x = x, Beta = 0.90, side = 1, upper = NULL, lower =
 NULL)



```
set.seed(100)
x \leftarrow rlogis(100, 5, 1)
out1 <- npbetol.int(x = x, Beta = 0.90, side = 1,
               upper = NULL, lower = NULL)
out2 <- npbetol.int(x = x, Beta = 0.90, side = 2,
               upper = NULL, lower = 4)
> out1
 beta 1-sided.lower 1-sided.upper
         3.486409
1 0.9
                     7.085171
> out2
 beta 2-sided.lower 2-sided.upper
1 0.9
                     7.563949
```





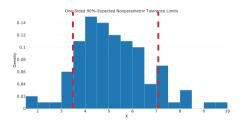


Figure: 1-Sided

```
plotly.plottol.hist(out1 , x=x , side = "two" ,
                    x.lab = "X", tol.lwd = 18.
                    x.lab.size = 36, x.tick.size=36.
                    y.lab.size = 36 , y.tick.size = 36 ,
                    title.size = 36 , title.position.y = 0.995)
_ College of Arts
                           University of North Carolina
```

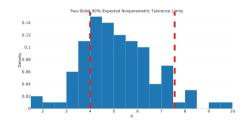


Figure: 2-Sided (with Lower Bound 4)

```
plotly.plottol.hist(out2 , x=x , side = "two" ,
                    x.lab = "X". tol.lwd = 18.
                    x.lab.size = 36, x.tick.size=36,
                    v.lab.size = 36 . v.tick.size = 36 .
                    title.size = 36 . title.position.v = 0.995)
```

Sample Size Determination: np.order

```
np.order(m, alpha, P, indices = (FALSE,TRUE))
```

Description:

np.order For given values of m, alpha, and P, this function solves the necessary sample size such that the r^{th} (or $(n-s+1)^{th}$) order statistic is the $[(1-\alpha)100\%,(P)100\%]$ lower (or upper) tolerance limit. This function can also report all combinations of order statistics for 2-sided intervals.





Sample Size Determination: np.order

Examples:

- Sample Size Only:
 np.order(m = 5, alpha = 0.05, P = 0.95, indices = FALSE)
- Sample Size With Indices:
 np.order(m = 5, alpha = 0.05, P = 0.95, indices = TRUE)



Sample Size Determination: np.order





Nonparametric Tolerance Interval: Application

Hamedani (2013) provided an application of survival times of 121 patients with breast cancer obtained from a large hospital in a period from 1929 to 1938.

Suppose we do not wish to impose any distributional assumption on the data. If tolerance limits are desired, nonparametric and therefore nptol.int can be applied under this situation.





Nonparametric Tolerance Interval: Application

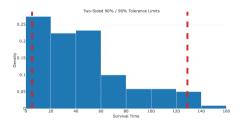


Figure: "WILKS"'s Method

The 2-sided $(P,\gamma)=(0.90,0.90)$ nonparametric tolerance limits using "WILKS"'s method is $(5\ ,\ 129).$





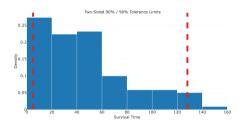


Figure: "YM"'s Method

The 2-sided $(P,\gamma)=(0.90,0.90)$ nonparametric tolerance limits using "YM"'s interpolation/extrapolation scheme is $(5\ ,\ 128.157).$

Regression Tolerance Interval

Regression Tolerance Intervals

- Introduction
- (Multiple) Linear Regression Tolerance Intervals: [regtol.int/regtol.int2]
- Nonlinear Regression Tolerance Interval: [nlregtol.int/nlregtol.int2]
- Nonparametric Regression Tolerance Interval: [npregtol.int/npregtol.int2]
- Application





Regression Tolerance Interval: Introduction

tolerance provides tools calculating tolerance limits for not only various univarite data, but also multivariate data and for regression settings.

More specifically, tolerance includes three functions regtol.int, nlregtol.int and npregtol.int for linear regression, nonlinear regression and nonparametric regression tolerance limits, respectively.

In addition, plottol and its updated version plotly.plottol.reg provides visualizations for tolerance limits under regressional settings.



```
regtol.int(reg, new.x, side = c(1,2), alpha, P)
```

Description:

regtol.int provides 1-sided or 2-sided (multiple) linear regression tolerance bounds. It is also possible to fit a regression through the origin model.

<u>Note:</u> we also update the original function to regtol.int2. regtol.int2 reorganizes the output. In addition, a new argument new is added. When new=FALSE, regtol.int2=regtol.int. In the following, regtol.int2 is used for demonstration purpose.



Methodology:

A multiple linear regression model is defined as

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_{p-1} X_{p-1} + \varepsilon$$

where $\beta_0,\beta_1,\cdots,\beta_{p-1}$ are the p regressors, and $\varepsilon \overset{iid}{\sim} \mathcal{N}(0,\sigma^2)$. The one-sided (P,γ) regression tolerance limits for each observation i are given by

$$L = \hat{y}_i - \hat{\sigma} k_{1,i}$$
 ; $U = \hat{y}_i + \hat{\sigma} k_{1,i}$

where

$$k_{1,i} = \frac{t_{(n-p);(1-\alpha)}^*(\sqrt{n_i^*z_P^*})}{\sqrt{n_i^*}}$$

and $t^*_{d;(1-\alpha)}(\gamma)$ is the $(1-\alpha)^{th}$ quantile of a non-central t distribution with d degree of freedom and non-centrality parameter $\gamma,\,z^*_P$ is the P^{th} quantile of a standard normal distribution. In addition $n^*_i=\frac{\hat{\sigma^2}}{s.e.(\hat{y}_i)^2}$ such that $s.e.(\hat{y}_i)$ is the standard error of \hat{y}_i .





Methodology:

The two-sided (P,γ) regression tolerance limits for each observation i are given by

$$L = \hat{y}_i - \hat{\sigma}k_{2,i}$$
 ; $U = \hat{y}_i + \hat{\sigma}k_{2,i}$

where $k_{2,i}$ is estimated according to the formula in Krishnamoorthy and Mathew (2009) such that let f=n-p then

$$k_{2,i} = \sqrt{\frac{f\chi_{1;P}^2(\frac{1}{n_i^*})}{\chi_{f;\alpha}^2}}$$

where $\chi^2_{d;\alpha}(\delta)$ is the α^{th} quantile of a non-central χ^2 distribution with d degree of freedom and non-centrality parameter δ .





Examples:

- One-Sided (without new data): $regtol.int2(reg = lm(y \sim x))$, side = 1, alpha = 0.05, P = 0.95)
- Two-Sided (with new data): $\frac{\text{Two-Sided (with new data):}}{\text{regtol.int2(reg = lm}(y \sim x), \text{ new.x = data.frame(x = c(3, 6, 12)),}}$ side = 2, alpha = 0.05, P = 0.95)



```
set.seed(100)
x \leftarrow runif(100, 0, 10)
y \leftarrow 20 + 5*x + rnorm(100, 0, 3)
out1 <- regtol.int2(reg = lm(v ~ x).
                     side = 1, alpha = 0.05, P = 0.95, new=TRUE)
out2 <- regtol.int2(reg = lm(y \sim x), new.x = data.frame(x = c(3, 6, 12)),
                     side = 2, alpha = 0.05, P = 0.95, new=TRUE)
out1
out2
```





regtol.int versus regtol.int2

regtol.int

- **1** One output $(\alpha, P, y, \hat{y}, Tls)$
- **2** Redundant information of (α, P)
- **3** Ordered by $\hat{y}'s$
- lacktriangle New data are ordered by estimated \hat{y}
- Does not include regtol.int2





regtol.int2

- Multiple outputs $(\$tol,\$\alpha.P.side,\$model,\$newdata)$
- More informative
- Ordered by original data (visualization friendly)
- New data are attached to the original data at the end
- Includes regtol.int

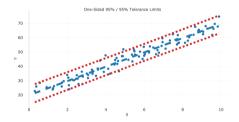


Figure: 1-Sided

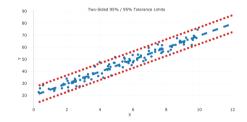


Figure: 2-Sided (with new data)

```
nlregtol.int(formula, xy.data, x.new = NULL, side = c(1,2), alpha, P,
maxiter = 50, ...)
```

Description:

nlregtol.int provides 1-sided or 2-sided nonlinear regression tolerance bounds.

Note:

- "..." are optional arguments passed to nls when estimating the nonlinear regression equation.
- we also update the original function to nlregtol.int2. nlregtol.int2 reorganizes the output. In addition, a new argument new is added. When new=FALSE, nlregtol.int2=nlregtol.int. In the following, nlregtol.int2 is used for demonstration purpose.





Methodology:

A nonlinear regression model is used to model the nonlinear relationship between a response variable Y with a given set of predictor variable X_1, \cdots, X_p . The nonlinear regression model is defined as

$$Y = f(\beta, X_1, \cdots, X_p) + \varepsilon$$

where β is a vector of regression parameters and ε is an error term following a specified distribution which is not necessarily normal.

Estimation of $\hat{y}_i's$ is done through nonlinear square routine.



Methodology:

The (P,γ) nonlinear regression tolerance limits are constructed in a similar manner as for the linear regression case. The only difference is how the effective sample size n_i^* is calculated.

For the nonlinear setting, n_i^* is a function of the partial derivatives of $f(\beta, x_{i,1}, \dots, x_{i,p})$ with respect to each of theregression parameters.

Further technical details can be found in Wallis (1951).





Examples:

- One-Sided (without new data):
 nlregtol.int2(formula = formula, xy.data = data.frame(cbind(y, x)), side = 1, alpha = 0.05, P = 0.95, new = TRUE)
- Two-Sided (with new data):
 nlregtol.int2(formula = formula, xy.data = data.frame(cbind(y, x)), x.new=cbind(c(10, 55)), side = 2, alpha = 0.05, P = 0.95, new = TRUE)



```
set.seed(100)
x \leftarrow runif(50, 5, 45)
f1 \leftarrow function(x, b1, b2) b1 + (0.49 - b1)*exp(-b2*(x - 8)) +
  rnorm(50, sd = 0.01)
v \leftarrow f1(x, 0.39, 0.11)
formula <- as.formula(y \sim b1 + (0.49 - b1)*exp(-b2*(x - 8)))
out1 <- nlregtol.int2(formula = formula,
                      xy.data = data.frame(cbind(y, x)), side = 1,
                      alpha = 0.05, P = 0.95, new = TRUE)
out2 <- nlregtol.int2(formula = formula,
                      xy.data = data.frame(cbind(y, x)),
                      x.new=cbind(c(10, 55)), side = 2,
                      alpha = 0.05, P = 0.95, new = TRUE
```





nlregtol.int versus nlregtol.int2

nlregtol.int

- One output $(\alpha, P, y, \hat{y}, Tls)$
- **2** Redundant information of (α, P)
- **3** Ordered by y's
- Does not include nlregtol.int2

nlregtol.int2

- Multiple outputs $(\$tol,\$\alpha.P.side,\$model,\$original.data)$
- More informative
- Ordered by original data (visualization friendly)
- Includes nlregtol.int





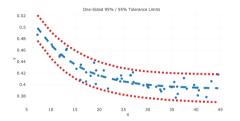


Figure: 1-Sided

Dr. Bing Zhang Department of Statistics

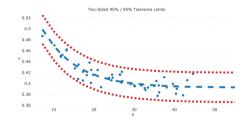


Figure: 2-Sided (with new data)

```
npregtol.int(x, y, y.hat, side = c(1,2), alpha, P, method =
c("WILKS", "WALD", "HM"), upper = NULL, lower = NULL)
```

Description:

npregtol.int provides 1-sided or 2-sided nonparametric regression tolerance bounds.

<u>Note:</u> we also update the original function to npregtol.int2. npregtol.int2 reorganizes the output. In addition, a new argument new is added. When new=FALSE, npregtol.int2=npregtol.int. In the following, npregtol.int2 is used for demonstration purpose.





Methodology:

A nonparametric regression model is used to model the nonlinear relationship between a response variable Y with a given set of predictor variables X_1, \dots, X_p but without parameters.

The nonparametric regression model is defined as

$$Y = f(X_1, \cdots, X_p) + \varepsilon$$

which is free of any parameters and arepsilon is a random error term which is only assumed to have mean 0.

Tolerance limits for nonparametric regression can be constructed based on order statistics of residuals, that is it is necessary to find $\hat{\varepsilon}_{[r]}$ and $\hat{\varepsilon}_{[s]}$. The corresponding (P,γ) upper and lower nonparametric regression tolerance limits are

$$L = \hat{y}_i + e_{[r]}$$
 ; $U = \hat{y}_i + e_{[s]}$

Method to determine r and s are given in *nonparametric tolerance intervals* section.





Examples:

- One-Sided (without limit specifications):
 npregtol.int2(x = x, y = y, y.hat = y.hat, side = 1, alpha =
 0.05. P = 0.95, method = "WILKS", new=TRUE)
- Two-Sided (with limit specifications):
 npregtol.int2(x = x, y = y, y.hat = y.hat, side = 2, alpha =
 0.05, P = 0.95, method = "WILKS", new=TRUE, lower = 0.38,
 upper=0.49)



```
set.seed(100)
x \leftarrow runif(50, 5, 45)
f1 \leftarrow function(x, b1, b2) b1+(0.49-b1)*exp(-b2*(x-8))+rnorm(50,sd = 0.01)
y \leftarrow f1(x, 0.39, 0.11)
v.hat <- loess(v~x)$fit
out1 <- npregtol.int2(x = x, y = y, y.hat = y.hat, side = 1,
                        alpha = 0.05, P = 0.95, method = "WILKS", new=TRUE)
out2 <- npregtol.int2(x = x, y = y, y.hat = y.hat, side = 2,
                        alpha = 0.05, P = 0.95, method = "WILKS".new=TRUE.
                        lower = 0.38 , upper=0.49)
0111.1
0111.2
```





npregtol.int versus npregtol.int2

npregtol.int

- One output $(\alpha, P, y, \hat{y}, Tls)$
- **2** Redundant information of (α, P)
- **3** Ordered by $\hat{y}'s$
- If a certain limit is set, it is hard to track purely based on output
- Ooes not include npregtol.int2





npregtol.int2

- Multiple outputs (\$tol,\$\alpha.P.side,\$method,\$lower.upper)
- More informative
- Ordered by original data (visualization friendly)
- Specified limits are reminded in the output
- Includes npregtol.int

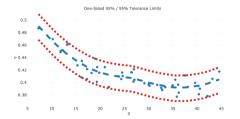


Figure: 1-Sided

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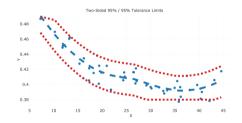


Figure: 2-Sided (with specified limits)

Regression Tolerance Interval: Application

Hospitals frequently study factors that are likely related to infections patients gain while hospitalized. Neter, Kutner, Nachtsheim, and Wasserman (1996) provided patients' infection data from a study of $n=113~{\rm US}$ hospitals.

Numerous variables are available to study, but a parsimonious multiple linear regression model is one that has infection risk as the response, and average length of patient stay and number of x-rays given by the hospital as predictors.





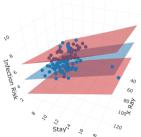
Regression Tolerance Interval: Application

The linear regression model in this application is

Infection Risk =
$$\beta_0 + \beta_1 X Ray + \beta_2 Stay + \varepsilon$$

For a dataset with 2 predictor regressors, a (P,γ) tolerance plane shall be generated.

Two-Sided 90% / 90% Tolerance Planes







Multivariate Tolerance Regions

Multivariate Tolerance Regions

- Introduction
- Multivariate Normal Tolerance Regions [mvtol.region]
- Multivariate Linear Regression Tolerance Regions [mvregtol.region]
- Application



Multivariate Tolerance Region: Introduction

Think of a situation where a quality engineer wishes to assess both the thickness and the diameter of a metal ring. Two elements are involved at the same time and they follow a bivariate (or multivariate) normal distribution approximately.

tolerance provides the option to calculate tolerance regions for multivariate normal distribution.



Methodology

A random vector $\mathbf{X} = (X_1, \cdots, X_p)^T$ follows a multivariate normal distribution if it has the density function

$$f_{\mathbf{X}}(\mathbf{x}, \mu, \Sigma) = \frac{1}{(2\pi)^{p/2} |\sigma|^{1/2}} e^{-(1/2)||\Sigma^{-1/2}(\mathbf{x} - \mu)||^2}$$

where $\mathbf{x} \in \mathbb{R}^p$, $\mu \in \mathbb{R}^p$, and Σ is a $p \times p$ symmetric and positive-definite matrix, and $||\mathbf{A}||^2 = \mathbf{A}^T \mathbf{A}$ for any matrix \mathbf{A} .

Normal tolerance regions require estimates of both μ and Σ , such that

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_{i} \quad ; \quad \hat{\mathbf{\Sigma}} = \frac{1}{n-1} \sum_{i=1}^{n} (\mathbf{x}_{i} - \hat{\mu})(\mathbf{x}_{i} - \hat{\mu})^{T}$$





Methodology

A (P, γ) normal tolerance region is given by

$$\mathbf{x} : ||S^{-1/2}(\mathbf{x}_i - \hat{\mu})||^2 < c$$

where c is the tolerance factor to be determined such that

$$\mathbb{P}[\mathbb{P}_{\mathbf{X}}\{||S^{-1/2}(\mathbf{x}_i - \hat{\mu})||^2 \le c; \mathbf{x}, S\} \ge P] = 1 - \alpha$$

To obtain the tolerance region, obtaining c is a critical step. For more technical details of how to calculate c based on Monte Carlo algorithm, please see Krishnamoorthy and Mondal (2006).



Multivariate Tolerance Regions: mvtol.region

```
mvtol.region(x, alpha, P, method = c("KM", "AM", "GM", "HM", "MHM",
"V11", "HM.V11", "MC", B, M))
```

Description:

mvtol.region determines the appropriate tolerance factor for computing multivariate normal tolerance regions based on Monte Carlo methods or other approximations.

Note:

- ▶ B is the number of iterations used for the Monte Carlo algorithms (i.e., when method = c("KM", "MC")), which determines the tolerance factor.
- ► M is the number of iterations used for the inner loop of the Monte Carlo algorithm specified through method = "MC".





Multivariate Tolerance Regions: mvtol.region

Bivariate Data

Trivariate Data





Multivariate Tolerance Regions: mvtol.region

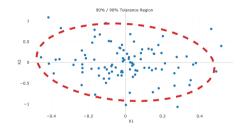


Figure: Bivariate

```
plotly.plottol.multi(out1, x , x.lab = "X1" , y.lab = "X2", x.cex=22,tol.lwd=18,tol.line.type="dot", x.tick.size = 36 , x.lab.size = 36, y.tick.size = 36 , y.lab.size = 36, title.size = 36 , title.position.y = 0.995)

and Sciences

ACHIEVIII F
```

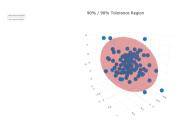


Figure: Trivariate

Multivariate Regression Tolerance Regions: mvregtol.region

```
mvregtol.region(mvreg, new.x, alpha, P, B))
```

Description:

mvregtol.region determines the appropriate tolerance factor for computing multivariate (multiple) linear regression tolerance regions based on Monte Carlo simulation.

Note:

▶ B The number of iterations used for the Monte Carlo algorithm which determines the tolerance factor. The number of iterations should be at least as large as the default value of 1000.





Multivariate Regression Tolerance Regions: mvregtol.region

Example:

```
## 95%/95% multivariate regression tolerance factors using
## a fertilizer data set presented in Anderson (2003, p. 374).
grain \leftarrow c(40, 17, 9, 15, 6, 12, 5, 9)
straw <- c(53, 19, 10, 29, 13, 27, 19, 30)
fert <- c(24, 11, 5, 12, 7, 14, 11, 18)
DF <- data.frame(grain.straw.fert)</pre>
new.x \leftarrow data.frame(fert = c(10, 15, 20))
mvreg <- lm(cbind(grain, straw) ~ fert + I(fert^2), data = DF)</pre>
set.seed(100)
out <- mvregtol.region(mvreg, new.x = new.x, alpha = 0.05,
                        P = 0.95, B = 5000
out
```





Multivariate Regression Tolerance Regions: mvregtol.region

Output:

```
> out
      k.factor grain.hat straw.hat fert I(fert^2)
                           51.34292
X 1
     24.962794 36.753376
                                       24
                                                 576
X2
      8.748968
                8.835535
                           20.31933
                                       11
                                                 121
ХЗ
                                                  25
     17.032422 10.200785
                           10.69490
Х4
      8.845872
                           22.21164
                9.483019
                                       12
                                                 144
Х5
     10.076046
                8.745673
                           13.57363
                                                  49
X6
                           26.24332
                                       14
      9.184379 11.528007
                                                 196
X7
      8.791323
                8.835535
                           20.31933
                                       11
                                                 121
X8
      9.725227 18.618069
                           35, 29492
                                       18
                                                 324
X1.1
      8.569849
                8.438059
                           18.50938
                                       10
                                                 100
X2.1
      9.468488 12.925512
                           28.38269
                                       15
                                                 225
X3.1 10.514037 23.663143
                           40.31484
                                       20
                                                 400
```





- Kidney function laboratory tests include a urinalysis to screen for the presence of protein and blood in the urine, a blood urea nitrogen (BUN) test to check for waste product in the urine, and a test to obtain the estimated glomerular filtration rate (eGFR), which is used to detect the presence and cause of kidney disease.
- Little information is available regarding normal reference values for kidney function in adolescents, which impacts how physicians diagnose and manage diabetes in this population.
- The reference population studied is healthy US adolescents between 12 and 17 years of age, with a number of criteria used to determine "healthy".
- We will construct nonparametric $(P,\gamma)=(0.95,0.95)$ semi-space rectangular tolerance regions to represent the reference regions of normal adolescent kidney function; we will look at the males in this sample, yielding n = 2529 subjects in the reference sample.



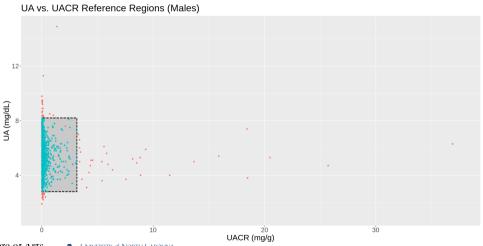


Methodology: In this application, a multivariate tolerance region is constructed using hyper-rectangle method developed by Young and Mathew (2020). An overview of the method is illustrated as follows:

- Calculate the data depth depth value of each observation;
- ② Trim the observations based on their data-depth value to capture at least a proportion of P sampled population at (1α) confidence level.
- $oldsymbol{\circ}$ Obtain the rectangle(s) which include(s) the inclusive observation to obtain the (P,γ) tolerance region. The region is expected to be in a hyper-rectangle shape.

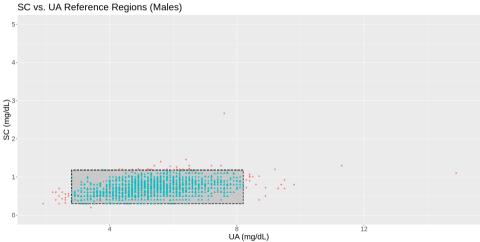






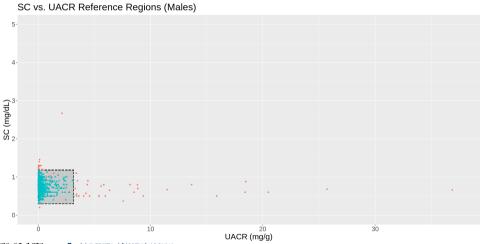
















Final Comments





Some Other Applications Using tolerance

- ▶ Used to construct tolerance intervals for establishing a pass/fail criterion of radiation portal monitors. [Burr and Gavron (2012), "Pass/Fail Criterion for a Simple Radiation Portal Monitor Test ." Modern Instrumentation; 1(3):27–33.]
- ▶ Used to help the design verification process of the Vagus Nerve Stimulation (VNS) Therapy system, which is FDA-approved for the treatment of refractory epilepsy and treatment-resistant depression. [Young et al. (2016), "Sample Size Determination Strategies for Normal Tolerance Intervals Using Historical Data." *Quality Engineering*; 28(3):337–351.]
- ▶ Used in molecular lymph node analysis to aid in the understanding of prostate cancer. [Heck et al. (2018), "Molecular Lymph Node Status for Prognostic Stratification of Prostate Cancer Patients Undergoing Radical Prostatectomy with Extended Pelvic Lymph Node Dissection." Clinical Cancer Research; 24(10):2342–2349.]
- ▶ Used to develop nonparametric and normal-based tolerance intervals on GH-2000 to detect doping in competitive sports. [Liu et al. (2021), "Comparison of Normal Distribution-Based and Nonparametric Decision Limits on the GH-2000 Score for Detecting Growth Hormone Misuse (Doping) in Sport." *Biometrical Journal*; 63(1):187–200.]





Recent and Forthcoming Additions to tolerance

Recent Additions

- ► Launched GitHub repo (https://github.com/dsy109/tolerance)
- ► Launched Shiny app (https://tolerance.as.uky.edu/)
- ► Added new graphics capabilities based on ggplot2 and plotly

Forthcoming Additions

- ▶ Improve efficiency of exact normal k-factor calculations using Rcpp
- ► Expanding the suite of regression-based tolerance intervals; e.g., simultaneous tolerance intervals and spatial regression tolerance regions
- ► Recording a training module; make available on my website

Open Discussion

As current (or future) end-users of the tolerance package, what are features that would be helpful for your research and data analysis needs?





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