Weibull Prediction Intervals for a Future Number of Failures

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September 26, 2000

Abstract

This paper evaluates exact coverage probabilities of approximate prediction intervals for the number of failures that will be observed in a future inspection of a sample of units, based only on the results of the first in-service inspection of the sample. The failure-time of such units is modeled with a Weibull distribution having a given shape parameter value. We illustrate the use of the procedures by using data from a nuclear power plant heat exchanger. The results suggest that the likelihood-based prediction intervals perform better than the alternatives.

Key Words: Coverage probability, Prediction bounds, Reliability prediction, Weibull distribution

1 Introduction

1.1 Motivation

Based on the number of failures found in a previous inspection of a group of in-service units, Nelson (1995, 2000) provides prediction limits for the additional number of failures that will be observed during a future time period. Nelson's intervals were motivated by the following application. Nuclear power plants contain large heat exchangers that transfer energy from the reactor to steam turbines. Such exchangers typically have 10,000 to

20,000 stainless steel tubes that conduct the flow of steam. Due to stress and corrosion, the tubes develop cracks over time. Cracks are detected during planned inspections. The cracked tubes are subsequently plugged to remove them from service. To develop efficient inspection and plugging strategies, the plant management can use a prediction of the added number of tubes that will need plugging by a specified future time. A prediction expressed as an interval indicates the magnitude of the possible prediction error and quantifies the "confidence" in the prediction.

1.2 Related work

There is a large amount of literature describing various statistical prediction applications and methods. Hahn and Nelson (1973), Patel (1989), and Chapter 5 of Hahn and Meeker (1991) provide surveys of methods for statistical prediction for a variety of situations.

For applications involving failure-time with censored data (as opposed to the single inspection available in our motivating example) methods presented by Lawless (1973), Nelson (1982), Mee and Kushary (1994), and Escobar and Meeker (1999) are useful. These previously developed prediction methods cannot be used for the kind of inspection data considered here.

1.3 Overview

Section 2 describes the "within-sample" prediction problem and presents a statistical model for it. Section 3 provides a general discussion of the coverage probabilities used to evaluate statistical prediction bounds or intervals. Section 4 provides procedures for constructing Nelson's (1995, 2000) prediction intervals based on confidence limits for the ratio of multinomial proportions and also on a likelihood ratio approach. This section also discusses issues related to specifying the Weibull shape parameter. Section 5 illustrates the use of Nelson's (1995, 2000) prediction interval procedures with an example, including an evaluation of sensitivity to deviations from the given Weibull shape parameter. Section 6 outlines computation of the actual coverage probabilities used to compare the prediction interval procedures. Section 7 discusses the design of an analytical experiment to evaluate the procedures and summarizes the results of the experiment. Section 8 provides suggestions for use of the prediction intervals in application and contains some concluding remarks. The Appendix provides some technical results on the behavior of the prediction interval procedures.

2 Model

2.1 Prediction problem

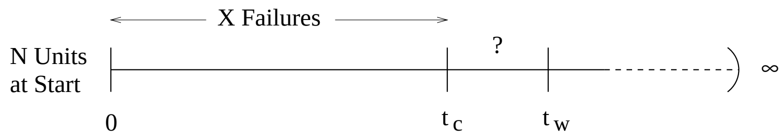

Figure 1: Within-sample prediction.

Suppose that N sample units start service at time 0, and that, by some censoring time t_c, the cumulative number of failures is X. We would like a prediction interval for the future added number Y of units that will fail by time t_w (e.g., end of a warranty period). That is, Y is the number of failures in the interval (t_c, t_w). If Z is the remaining number of unfailed units at time t_w, then (X, Y, Z) will have a trinomial distribution with corresponding probabilities (p, q, r), where $X + Y + Z = N$ and $p + q + r = 1$. Figure 1 illustrates the within-sample prediction problem.

2.2 Weibull distribution

The probabilities p, q, and r depend on the assumed failure-time distribution. For Nelson's (2000) prediction limits, it is assumed that the failure times are independent observations from a Weibull distribution with unknown scale parameter η and given ("known") shape parameter β. Thus,

$$\begin{aligned}
p &= 1 - \exp\left[-(t_c/\eta)^{\beta}\right] \\
q &= \exp\left[-(t_c/\eta)^{\beta}\right] - \exp\left[-(t_w/\eta)^{\beta}\right] \qquad (1) \\
r &= \exp\left[-(t_w/\eta)^{\beta}\right].
\end{aligned}$$

3 Coverage probability for statistical prediction interval procedures

Following Nelson (2000), our goal is to predict the number of additional failures Y in a future interval based on earlier information from the same sample. The cumulative number of failures X observed before the censoring time t_c can be used to obtain an approximate prediction interval with nominal confidence level $1-\alpha$, denoted by $PI(1-\alpha) = [\underset{\sim}{Y}_x, \quad \tilde{Y}_x]$. With any sensible procedure for generating such an interval, including those given in Section 4, both $\underset{\sim}{Y}_x$ and $\tilde{Y}_x$ will be nonnegative integers. The future random variable Y and $[\underset{\sim}{Y}_x, \quad \tilde{Y}_x]$ have a joint distribution that depends on the unknown scale parameter η.

3.1 Coverage probability for two-sided prediction intervals

It is important to distinguish between two types of coverage probabilities:

- Conditioned on X, the number of additional failures, Y, has a BINOMIAL$(N-X, \pi)$ distribution, where

$$\pi = \frac{q}{q+r} \tag{2}$$

  is a function of the probabilities q and r from (1); π is the conditional probability that a sample unit fails in the interval (t_c, t_w), given that it survived until t_c. We denote the above conditional binomial cdf as $\Pr(Y \le y \mid X) = \text{BINCDF}(y, N-X, \pi)$.

  For given X and resulting $[\underset{\sim}{Y}_x, \quad \tilde{Y}_x]$, the conditional coverage probability of the specific prediction interval with nominal confidence level $1-\alpha$ is

$$\begin{aligned} \text{CP}[PI(1-\alpha) \mid X; \eta] &= \Pr(\underset{\sim}{Y}_x \le Y \le \tilde{Y}_x \mid X; \eta) \\ &= \text{BINCDF}(\tilde{Y}_x, N-X, \pi) - \text{BINCDF}(\underset{\sim}{Y}_x - 1, N-X, \pi). \end{aligned} \tag{3}$$

  The actual conditional coverage probability in (3) is random because $[\underset{\sim}{Y}_x, \quad \tilde{Y}_x]$ depends on X, which varies from sample to sample. This probability is also unknown here, because π depends on the unknown scale parameter η.

- One is generally interested in evaluating the coverage probability associated with a prediction interval *procedure*. The unconditional coverage probability (for a procedure) is the expected value of the conditional coverage probability in (3) with respect to the random variable X; that is,

$$\begin{aligned} \mathrm{CP}[PI(1-\alpha);\eta] &= \Pr(\underset{\sim}{Y}_x \leq Y \leq \tilde{Y}_x;\eta) \\ &= \mathrm{E}_X\left\{\mathrm{CP}[PI(1-\alpha)\mid X;\eta]\right\}. \end{aligned} \tag{4}$$

3.2 Relationship between two-sided prediction intervals and one-sided prediction bounds

A two-sided $100(1-\alpha)\%$ prediction interval may be obtained by combining a one-sided lower $100(1-\alpha_1)\%$ prediction bound and a one-sided upper $100(1-\alpha_2)\%$ prediction bound, where $\alpha_1+\alpha_2=\alpha$. By using equal-tail prediction intervals (i.e., $\alpha_1=\alpha_2=\alpha/2$), both end points of the resulting interval can be interpreted as one-sided prediction bounds (after making the necessary adjustment in the confidence level). Escobar and Meeker (1999, Section 2.3) provide more discussion of the coverage probabilities for statistical prediction intervals and one-sided bounds.

4 Prediction and prediction limits

4.1 Point prediction

It may be desirable to have a single prediction $\widehat{Y}$ for the number of additional failures Y in a future interval (t_c, t_w). Given the observed (nonzero) number of failures X by t_c, the maximum likelihood (ML) estimate of η is

$$\widehat{\eta} = \frac{t_c}{(-\log[1-(X/N)])^{1/\beta}}. \tag{5}$$

As suggested by Nelson (2000), the corresponding point prediction for Y is

$$\widehat{Y} = N \times \widehat{q}, \tag{6}$$

where the estimate $\widehat{q}$ is obtained by substituting $\widehat{\eta}$ into (1) for q, yielding

$$\widehat{q} = [1-(X/N)] - [1-(X/N)]^{(t_w/t_c)^\beta}. \tag{7}$$

While the point prediction provides a "best guess" for the future realization of the random variable Y based the observed value of X, it does not give any indication of prediction precision and is therefore much less informative than a prediction interval.

4.2 Prediction bounds: probability ratio (PR) procedure

Following Nelson (2000), when the Weibull probabilities p and q are small, the approximation

$$\begin{aligned} \frac{q}{p} &= \frac{\left(1 - \exp\left[-(t_w/\eta)^\beta\right]\right) - \left(1 - \exp\left[-(t_c/\eta)^\beta\right]\right)}{1 - \exp\left[-(t_c/\eta)^\beta\right]} \\ &\approx \frac{(t_w/\eta)^\beta - (t_c/\eta)^\beta}{(t_c/\eta)^\beta} \\ &= (t_w/t_c)^\beta - 1 \end{aligned} \tag{8}$$

does not depend on the unknown Weibull scale parameter η. Nelson (1972) gives a conservative $100(1-\alpha)\%$ confidence interval for the trinomial probability ratio p/q as $[g_{\mathrm{L}}(Y, X, \alpha_1), \quad g_{\mathrm{U}}(Y, X, \alpha_2)]$, where

$$g_{\mathrm{L}}(Y, X, \alpha_1) = \begin{cases} X/[(Y+1)\mathcal{F}(1-\alpha_1, 2Y+2, 2X)] & X \neq 0 \\ 0 & X = 0 \end{cases} \tag{9}$$

and

$$g_{\mathrm{U}}(Y, X, \alpha_2) = [(X+1)\mathcal{F}(1-\alpha_2; 2X+2, 2Y)]/Y. \tag{10}$$

Here $\mathcal{F}(\gamma; m, n)$ is the γ quantile of the $\mathcal{F}$ distribution with m numerator degrees of freedom and n denominator degrees of freedom, and $\alpha_1 + \alpha_2 = \alpha$. As before, X and Y denote the number of failures in the intervals $(0, t_c]$ and (t_c, t_w), respectively. The justification for this interval is that

$$\Pr\left(g_{\mathrm{L}}(Y, X, \alpha_1) \leq \frac{p}{q} \leq g_{\mathrm{U}}(Y, X, \alpha_2)\right) \geq 1 - \alpha,$$

as shown in the appendix of Nelson (1972) and in Nelson (2000).

Then, using the approximation in (8) for small p and q, the above limits will provide an approximate $100(1-\alpha)\%$ confidence interval for $\left[(t_w/t_c)^\beta - 1\right]^{-1}$; that is,

$$\Pr\left(g_{\mathrm{L}}(Y, X, \alpha_1) \leq \frac{1}{(t_w/t_c)^\beta - 1} \leq g_{\mathrm{U}}(Y, X, \alpha_2)\right) \approx 1 - \alpha. \tag{11}$$

Given the (nonzero) number of failures X and $0 < \alpha < 1$, both $g_{\mathrm{L}}(y, X, \alpha)$ and $g_{\mathrm{U}}(y, X, \alpha)$ are monotonically decreasing functions of positive, real-valued y. Hence, the "floor" of smallest, positive real y-value that satisfies the left inequality in (11) is an approximate one-sided lower $100(1-\alpha_1)\%$

prediction bound for Y. We denote this bound by $\underset{\sim}{Y}_{\text{pr}}$. If $X = 0$, we may only produce a trivial lower bound for the number of failures in (t_c, t_w). We define $\underset{\sim}{Y}_{\text{pr}}$ to be zero in this case.

The "ceiling" of the largest real y-value that satisfies the right inequality in (11) is an approximate one-sided upper $100(1-\alpha_2)\%$ prediction bound for Y, denoted by $\tilde{Y}_{\text{pr}}$. Together $\underset{\sim}{Y}_{\text{pr}}$ and $\tilde{Y}_{\text{pr}}$ produce Nelson's (2000) approximate $100(1-\alpha)\%$ prediction interval $\left[\underset{\sim}{Y}_{\text{pr}}, \quad \tilde{Y}_{\text{pr}}\right]$ for Y.

Because $g_{\text{L}}(0, X \neq 0, \alpha_1) = X/\mathcal{F}(1-\alpha_1; 2, 2X)$, it is important to recognize that if $(t_w/t_c)^{\beta} - 1 \leq \mathcal{F}(1-\alpha_1; 2, 2X)/X$, the $100(1-\alpha_1)\%$ lower prediction bound $\underset{\sim}{Y}_{\text{pr}}$ will necessarily be zero; that is, all nonnegative integer y-values will then satisfy the left inequality in (11). In addition, depending on X, $(t_w/t_c)^{\beta}$, and the level of confidence (α_1 or α_2), the PR procedure may yield lower or upper prediction bounds that fall outside the sample space of Y (namely, bounds greater than $N - X$). The appendix describes these circumstances as well as some other technical details. If the computed value of $\tilde{Y}_{\text{pr}}$ is greater than $N - X$, we reset the upper bound to $N - X$. Likewise, if the PR procedure produces a lower prediction bound greater than $N - X$, we redefine the bound to be $N - X - 1$. Note also that, given X and the ratio $(t_w/t_c)^{\beta}$, the upper and lower prediction bounds provided by this procedure do not depend on the initial sample size N.

4.3 Simplified probability ratio (SPR) prediction bounds

As suggested by Nelson (2000), simpler multinomial probability ratio bounds for large Y result from noting that, (for fixed X) as $y \longrightarrow \infty$,

- $\mathcal{F}(1-\alpha_1; 2y+2, 2X)$ converges to $\mathcal{F}(1-\alpha_1; \infty, 2X) = 1/\mathcal{F}(\alpha_1; 2X, \infty) = 2X/\chi^2(\alpha_1; 2X)$, where $\chi^2(\gamma; n)$ denotes the γ quantile of a chi-square distribution with n degrees of freedom.

- $\mathcal{F}(1-\alpha_2; 2X+2, 2y)$ converges to $\mathcal{F}(1-\alpha_2; 2X+2, \infty) = \chi^2(1-\alpha_2; 2X+2)/(2X+2)$.

Substituting these limiting values for the $\mathcal{F}$ quantiles appearing on the left and right sides of (11) yields easy-to-compute, approximate one-sided lower $100(1-\alpha_1)\%$ and upper $100(1-\alpha_2)\%$ prediction bounds given by Nelson (2000):

$$\underset{\sim}{Y}_{\text{spr}} = \left\lfloor 0.5\left((t_w/t_c)^{\beta} - 1\right)\chi^2(\alpha_1; 2X) - 1\right\rfloor$$

and

$$\tilde{Y}_{\text{spr}} = \left\lceil 0.5 \left((t_w/t_c)^{\beta} - 1 \right) \chi^2(1 - \alpha_2; 2X + 2) \right\rceil, \qquad (12)$$

respectively. The floor and ceiling functions are represented above by $\lfloor\rfloor$ and $\lceil\rceil$. If $X = 0$ or if $0.5\left[(t_w/t_c)^{\beta} - 1\right]\chi^2(\alpha_1; 2X) < 1$, we define $\underset{\sim}{Y}_{\text{spr}}$ to be zero. The advantage of these intervals is that they can be computed directly without any iteration.

With X and α_1 fixed, if $\mathcal{F}(1-\alpha_1; 2y+2, 2X)$ is a decreasing (*increasing*) function of positive, real-valued y, the lower bound $\underset{\sim}{Y}_{\text{spr}}$ will be greater (*less*) than or equal to the previous probability ratio-based bound $\underset{\sim}{Y}_{\text{pr}}$ derived from (11). Similarly, the upper bound $\tilde{Y}_{\text{spr}}$ will be less (*greater*) than or equal to $\tilde{Y}_{\text{pr}}$ if $\mathcal{F}(1-\alpha_2; 2X+2, 2y)$ is a decreasing (*increasing*) function of y.

4.4 Prediction bounds: likelihood ratio (LR) procedure

The preceding prediction bounds are approximate and suitable for small p and q. Another approximate procedure suggested by Nelson (2000), which is appropriate for more general values of p and q, can be based on a likelihood ratio statistic as follows. The two-parameter multinomial likelihood for the observed (x, y, z) is

$$\mathcal{L}(p, q; x, y) = \mathcal{C} p^x q^y (1 - p - q)^{N-x-y}, \qquad (13)$$

where $\mathcal{C} = N!/(x!y!(N-x-y)!)$ is the multinomial coefficient. The maximum of (13) is

$$\mathcal{L}^*(x, y) = \mathcal{C}(x/N)^x (y/N)^y (1 - x/N - y/N)^{N-x-y}. \qquad (14)$$

Under the Weibull distribution model with probabilities (p, q, r) given by (1), the one-parameter constrained sample likelihood is

$$\mathcal{K}(\eta; x, y) = \mathcal{C}\left(1 - e^{-(t_c/\eta)^{\beta}}\right)^x \left(e^{-(t_c/\eta)^{\beta}} - e^{-(t_w/\eta)^{\beta}}\right)^y \left(e^{-(t_w/\eta)^{\beta}}\right)^{N-x-y}. \qquad (15)$$

The ML estimate $\widehat{\eta}(x, y)$ of the Weibull scale parameter must be found numerically by maximizing (15). We denote the maximum of (15) by $\mathcal{K}^*(x, y)$.

The log likelihood ratio test statistic comparing the constrained Weibull likelihood with the unconstrained multinomial likelihood is

$$\mathcal{Q}(x, y) = -2\left(\log\left[\mathcal{K}^*(x, y)\right] - \log\left[\mathcal{L}^*(x, y)\right]\right). \qquad (16)$$

If the true distribution is Weibull, then the asymptotic distribution of $\mathcal{Q}(X, Y)$ is approximately chi-square with 1 degree of freedom. Hence, for the random variables X and Y,

$$\Pr\left(\mathcal{Q}(X, Y) \leq \chi^2(1-\alpha; 1)\right) \approx 1 - \alpha. \tag{17}$$

Given the cumulative number of failures X by time t_c, the set of y-values for which $\mathcal{Q}(X, y) \leq \chi^2(1-\alpha; 1)$ provides an approximate $100(1-\alpha)\%$ prediction region for Y. In particular, the "floor" and "ceiling" of the respective smallest and largest positive real values that satisfy this inequality, say $\underset{\sim}{Y}_{\text{lr}}$ and $\tilde{Y}_{\text{lr}}$, yield the approximate $100(1-\alpha)\%$ likelihood ratio-based prediction interval for Y. A one-sided (lower or upper) $100(1-\alpha)\%$ prediction bound can be obtained from the appropriate end point of a two-sided $100(1-2\alpha)\%$ prediction interval.

4.5 Specification of the Weibull shape parameter

The prediction interval procedures described in Sections 4.2 to 4.4 are based on the assumption that a single group of units "on trial" is a random sample from a Weibull distribution with a given shape parameter, β. Of course, in applications, knowledge of β is inexact.

When prior information is available, a Bayesian approach may be useful. There can, however, be difficulties in some applications that would require the use of alternative methods. For the heat exchanger tubes, the Weibull shape parameter is not identifiable from the available data and thus the prior distribution for β would effectively determine the answer. Especially in such situations, sensitivity analysis to assess the effect of changes in an uncertain prior distribution is an essential part of the analysis. The one-parameter sensitivity analysis for the non-Bayesian prediction procedures given in Sections 4.2 to 4.4 would be more straightforward than a sensitivity analysis involving prior distributions for the Weibull distribution parameters.

When there has been a considerable amount of past experience with similar situations (material and failure mechanism combinations), it may be reasonable and safe to use a particular value for the Weibull shape parameter in decision making. For example, the shape parameter of a reliability distribution (reflecting spread on the log scale) also tends to be a function of material/device and failure mechanism. Such information is available in various places, including MIL-STD 217 and Klinger, Nakada, and Menendez (1990) who give tables of what are effectively Weibull parameters for different devices. Relatedly, Abernethy (1998) describes the use of a

"Weibull library" that contains information about past analyses that can be used to glean information on Weibull shape parameters for particular failure mode. Similar methods were advocated in Abernethy, Breneman, Medlin, and Reinman (1983).

When such engineering knowledge is used, it is important to conduct appropriate sensitivity analyses. Nelson (1985) discusses and illustrates the use of a given Weibull shape parameter for a different kind of reliability estimation problem and illustrates the use of sensitivity analysis to evaluate confidence bounds over a range of plausible shape parameter values.

5 An example: heat exchangers

For illustration, consider Nelson's (1995, 2000) example of a heat exchanger with $N = 20{,}000$ tubes. When inspected at age $t_c = 3$ years, $X = 8$ tubes had failed (i.e., had a crack initiation requiring that the tube be plugged). Suppose plant managers need a prediction and prediction bounds for the additional number Y of tubes that will need plugging by a future inspection at age $t_w = 10$ years.

The stress corrosion cracks in the heat exchanger are a phenomena that has been observed since the first nuclear power plants went into service. After many years of service, hundreds of the individual tubes in a given heat exchanger will develop cracks and be taken out of service, before the entire heat exchanger is retired. With that amount of experience and corresponding life data with previous heat exchangers, engineers would have a good basis for specifying some reasonable range of values for such a stress corrosion cracking shape parameter. Following Nelson (2000), to obtain the prediction, the Weibull shape parameter $\beta = 3.3$ is used. In practice, most engineers would choose such a value to be conservatively large (when extrapolating beyond the range of the data, larger values of β, indicating less spread in the distribution, will provide more pessimistic predictions, as we will see in our sensitivity analysis to follow).

Using (6) and the within-sample information, we would predict that $\widehat{Y} = 413$ additional tubes will fail in the next seven years, since

$$\begin{aligned}
\widehat{q} &= [1 - (8/20000)] - [1 - (8/20000)]^{(10/3)^{3.3}} \\
&= 0.0206396, \\
\widehat{Y} &= 20000(0.0206396) \\
&= 412.8.
\end{aligned}$$

Table 1: 90% prediction intervals for the added number of cracked heat exchanger tubes, assuming $N = 20{,}000$, $X = 8$, $t_c = 3$ years, $t_w = 10$ years.

Procedure		Shape parameter, β 3.0	3.3	3.6
Probability Ratio	$[\underset{\sim}{Y}_{\text{pr}}, \tilde{Y}_{\text{pr}}]$	[140, 524]	[205, 756]	[297, 1090]
Simplified PR	$[\underset{\sim}{Y}_{\text{spr}}, \tilde{Y}_{\text{spr}}]$	[142, 521]	[206, 753]	[298, 1087]
Likelihood Ratio	$[\underset{\sim}{Y}_{\text{lr}}, \tilde{Y}_{\text{lr}}]$	[148, 487]	[216, 700]	[311, 1001]

Table 1 provides equal-tail 90% prediction intervals for the added number of cracked tubes in the span of 3 to 10 years, based on the three procedures described in the previous section. Two additional values of the Weibull shape parameter are also used to evaluate the effect of misspecification of β on the prediction bounds. The prediction intervals are also shown graphically in Figure 2.

The intervals produced by the two probability ratio-based procedures agree closely, because the lower predictions for Y are fairly large. Substituting $X = 8$ and $\alpha_1 = \alpha_2 = .05$ into the $\mathcal{F}$ quantiles appearing in (9) and (10), it so happens that $\mathcal{F}(.95; 2y + 2, 16)$ and $\mathcal{F}(.95; 18, 2y)$ are both decreasing functions of positive, real-valued y. As mentioned earlier, this implies that the 90% prediction intervals from the probability ratio procedure in Section 4.2 should be wider than the intervals produced with the simplified probability ratio-based bounds (as seen in the Table 1 and Figure 2).

The PR and SPR intervals are wider than the LR intervals. This is related to results that will be described in the next section. In situations corresponding to this example (a similar number of tubes and fraction failing), the LR method tends to have coverage probability close to nominal, but the PR and SPR methods tend to be somewhat conservative, resulting in the longer intervals. Focusing on the likelihood ratio interval, the sensitivity analyses indicate that, even with the pessimistic value of $\beta = 3.6$, the number of failed tubes before the end of 10 years is unlikely to exceed 5% of the $N = 20{,}000$ tubes in the heat exchanger (heat exchangers are typically designed to have from 5% to 10% excess capacity to allow cracked tubes to be taken out of service without having to replace the entire heat exchanger).

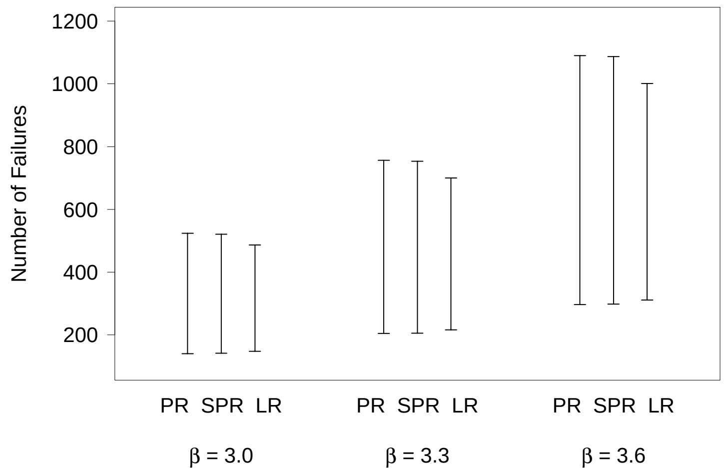

Figure 2: 90% prediction intervals for the added number of cracked heat exchanger tubes, assuming $N = 20{,}000$, $X = 8$, $t_c = 3$ years, $t_w = 10$ years.

6 Evaluation of coverage probabilities for each prediction interval procedure

As described in Section 3, we are interested in evaluating and comparing the unconditional coverage probabilities of prediction intervals (or prediction bounds) produced by each of Nelson's (2000) three procedures. The cumulative number of failures X by time t_c has a BINOMIAL(N, p) distribution and, conditioned on X, Y has a BINOMIAL$(N - X, \pi)$ distribution with the conditional probability $\pi = q/(1-p)$ from (2). Given a value of $0 \leq X \leq N - 1$, we use one of the procedures to construct an approximate $100(1-\alpha)\%$ lower or upper prediction bound, denoted by $\underset{\sim}{Y}_{X;\alpha}$ or $\tilde{Y}_{X;\alpha}$ [as a function of X and $(1-\alpha)$]. If $X = N$, there is no uncertainty in prediction because $\Pr(Y = 0) = 1$.

As suggested to us by Nelson in a private communication, the unconditional coverage probability of an approximate one-sided lower $100(1-\alpha)\%$ prediction interval can be computed analytically. The needed expressions are

$$\mathrm{CP}[PI(1-\alpha); N, p, q] \;=\; \sum_{k=0}^{N}\left[\Pr(X=k)\Pr\left(Y \geq \underset{\sim}{Y}_{k;\alpha} \mid X=k\right)\right]$$

$$= \sum_{k=0}^{N-1}\left[\binom{N}{k}p^k(1-p)^{N-k}\left(\sum_{j=\underset{\sim}{Y}_{k;\alpha}}^{N-k}\binom{N-k}{j}\pi^j(1-\pi)^{N-k-j}\right)\right] + p^N.$$

The coverage probability of the corresponding one-sided upper $100(1-\alpha)\%$ prediction interval can be found by replacing the inner summation above with

$$\Pr\left(Y \leq \tilde{Y}_{k;\alpha} \mid X=k\right) = \sum_{j=0}^{\tilde{Y}_{k;\alpha}}\binom{N-k}{j}\pi^j(1-\pi)^{N-k-j}.$$

For an observed value of X and a specified confidence level, both probability ratio-based procedures require only the factor $(t_w/t_c)^\beta$ to compute a prediction bound. This can be seen from (11). The likelihood ratio-based procedure requires specification of both $(t_w/t_c)^\beta$ and N.

The dependence of the likelihood procedure on the values of N and $(t_w/t_c)^\beta$ can be justified as follows. Any time scale can be transformed (divided by t_c) so that the "standardized" censoring time $t'_c = 1$, the "standardized" prediction time $t'_w = t_w/t_c$, and the "standardized" scale parameter $\eta' = \eta/t_c$; this re-scaling of time will not change the Weibull probabilities p, q, and r from (1) or the shape parameter β. The likelihood ratio-based procedure requires values for t_c, t_w, and β only when maximizing the constrained Weibull likelihood (15) with respect to η. Alternatively, we may obtain the same maximum value of (15) by optimizing with respect to $(\eta')^\beta$ on a t_c-transformed time scale once we know $(t'_w)^\beta$. Hence, besides the observed value of X, we need only specify N and $(t_w/t_c)^\beta$ to use the likelihood ratio procedure.

Noting that

$$(t_w/t_c)^\beta = \frac{\log(1-p-q)}{\log(1-p)},$$

we may completely determine an unconditional coverage probability for any of the three procedures by specifying a sample size N and values for the

Weibull probabilities p and q. These three "parameters" allow the computation of both a prediction interval given any $0 \leq X \leq N$ and the unconditional coverage probability (the expected value of the conditional coverage probabilities) for a procedure.

7 Comparison of Coverage Probabilities of the Prediction Procedures

7.1 Design of the analytical experiment

An analytical experiment was designed to study the effect that the following factors have on the coverage probability of the different prediction interval procedures.

- p: the (Weibull) probability that a sample unit fails by the censoring time, t_c.
- Np: the expected number of failures by t_c.
- q/p: the ratio of the true proportions failing in the intervals (t_c, t_w) and $(0, t_c]$, respectively.

We use this particular "parameterization" of (N, p, q) for two reasons: 1) each prediction interval procedure depends on the "known" quantity $(t_w/t_c)^{\beta} - 1$, which is an approximation of q/p by (8); 2) often with reliability data, the expected number of failures by the censoring time (i.e. Np) heavily influences the accuracy of large-sample approximations.

Any combination of the three above factors that results in plausible values for (N, p, q) [i.e. $0 < p < 1$, $q/p < (1-p)/p$, and $(Np)/p$ an integer] admits an unconditional coverage probability for a given prediction interval procedure. In our experiment, the level combinations used were $p = 0.05$, 0.005, 0.0005; $q/p = 1$, 10, 100; and $Np \in \{n/2 \mid n \in \mathbf{N}, n \leq 30 \text{ or } n = 10j, j = 4, \ldots, 10\}$. Note that having both $p = 0.05$ and $q/p = 100$ is impossible.

Interest focused on each procedure's coverage probability for one-sided prediction bounds, because most practical problems tend to be one-sided (with a prediction error on one side costing much more than on the other). We compare actual coverage probabilities with nominal values to assess the adequacy of the approximations.

Using formulas from Section 6, we calculated unconditional coverage probabilities for upper and lower approximate 95% prediction bounds produced with the likelihood ratio (LR), probability ratio (PR), and simplified

Table 2: $(t_w/t_c)^\beta$ for several values of p and q/p. The percent error in using $\left[(t_w/t_c)^\beta - 1\right]^{-1}$ to approximate p/q is shown inside parentheses.

		q/p		
		1	10	100
	0.05	2.054 (5.1)	15.567 (31.4)	–
p	0.005	2.005 (0.5)	11.286 (2.8)	140.288 (28.2)
	0.0005	2.000 (0.1)	11.028 (0.3)	103.613 (2.6)

probability ratio (SPR) procedures. A program was written in Fortran to compute all coverage probabilities with calculations performed in double precision. The accuracy of each calculated probability was approximately 5 significant digits.

7.2 Results of the analytical experiment

Various numerical and graphical methods were used to explore and summarize the results of the analytical study. We present a few of the most interesting and informative graphical displays.

Figure 3 shows plots of unconditional coverage probabilities for one-sided 95% prediction bounds (from the LR, PR, and SPR procedures) versus the expected number of failures (Np) by t_c when $p = 0.0005$ and $q/p = 1, 10, 100$. Figures 4 and 5 provide the same type of plots with $p = 0.005$ and $p = 0.05$, respectively. Table 2 shows the value of $(t_w/t_c)^\beta$ as determined by the factors p and q/p from each figure and also the percent error of the approximation $\left[(t_w/t_c)^\beta - 1\right]^{-1}$ for p/q (namely, $100 \times (1 - q/p\left[(t_w/t_c)^\beta - 1\right]^{-1})$).

Let LPB (UPB) denote a lower (upper) prediction bound. Some observations from Figures 3 to 5 and Table 2 are:

- With each procedure, the coverage probabilities of the one-sided bounds tend to oscillate as a function of Np. The fluctuation is most apparent when $Np \leq 10$ (and when q/p is large). This characteristic of the coverage probabilities is due to the conditional binomial distribution of Y given X, and it can be seen in other intervals involving discrete distributions. Agresti and Coull (1998) and Vollset (1993) present plots of coverage probabilities (for binomial parameter confidence intervals) that exhibit similar behavior.

- For the LR procedure, the coverage probabilities of both the LPBs and UPBs converge asymptotically and often quickly to the nominal

95% confidence level as Np increases (for all values of p and q/p). For each value of p in the figures, the rate of convergence to the nominal level grows as q/p increases (so that the expected number of failures in (t_c, t_w), namely Nq, becomes larger). This seems natural; as the expected number of failures increases, the large-sample approximation should be better.

- With the PR and SPR procedures, the coverage probability of the LPBs and UPBs is generally much closer to the nominal confidence level for small values of p and q.

- At each value of p, the coverage probabilities for the PR and SPR UPBs become quite conservative when q/p [and consequently $(t_w/t_c)^\beta$] assumes its highest level. These coverage probabilities often equal 1 in the two cases where $q = (q/p) \times p = 0.5$ and the approximation of p/q has the greatest percent error (from Table 2). The coverage probabilities of the corresponding LPBs drop, often far, below the nominal confidence level in the same situation. This indicates that, for each value of Np, both the PR and SPR procedures may produce strongly biased upward UPBs and LPBs on a region of X-values that has substantial probability.

- When q/p is largest for its corresponding level of p, the coverage probabilities associated with the PR and SPR procedures are nearly indistinguishable for both UPBs and LPBs; the procedures generate almost identical LPBs and UPBs. As described in Section 4.3, the bounds from both procedures will agree as the expected number of failures in the interval (t_c, t_w) increases.

- The LR LPBs always appear to be conservative. In cases where $q/p \geq 10$, the LR UPBs are anticonservative for $Np > 1$ and conservative for $Np \leq 1$. When $q/p = 1$, the UPBs from the LR procedure seem to be conservative.

- For every level of p, q/p, and Np, the coverage probabilities corresponding to the UPBs and LPBs from the PR procedure are at least as great as those of the SPR bounds. The approximate one-sided 95% PR prediction intervals tend to be wider than those from the SPR procedure.

- In general, the UPBs and LPBs from the LR procedure have coverage probabilities closer to the nominal confidence level than the bounds from the PR and SPR procedures.

For a given sample size N, the PR and SPR procedures will generally produce prediction bounds greater than $N - X$ for $X \geq X^*[(t_w/t_c)^\beta]$, an integer value that depends on the factor $(t_w/t_c)^\beta$. The appendix describes this event in detail. (In this case, we define the lower bounds, $\underset{\sim}{Y}_{\text{pr}}$ and $\underset{\sim}{Y}_{\text{spr}}$, to be $N - X - 1$ and the upper bounds, $\tilde{Y}_{\text{pr}}$ and $\tilde{Y}_{\text{spr}}$, to be $N - X$.) The LR procedure also will eventually (when X is sufficiently sizable) generate the lower and upper prediction bounds, $N - X - 1$ and $N - X$, but never bounds outside the range of Y. However, the PR and SPR procedures yield extreme bounds for much smaller values of X compared to the LR procedure. That is, there will often exist a subset of the sample space of X, of considerable probability, on which only the PR and SPR procedures will create prediction bounds outside the sample space of Y.

The quantity $\left[(t_w/t_c)^\beta - 1\right]^{-1}$ is always less than p/q (as the appendix shows) and the approximation error may be severe when either p or q is relatively large. For a fixed sample size, as $(t_w/t_c)^\beta$ increases and the approximation in (8) breaks down, $X^*[(t_w/t_c)^\beta]$ decreases to zero. In this situation, the PR and SPR bounds, both lower and upper, will become strongly biased upward. This may then reduce (*increase*) the actual coverage probability of the PR and SPR LPBs (*UPBs*). The potential danger of an inadequate approximation of p/q is demonstrated in the coverage probability plots for $(p, q/p) = (0.005,100)$ and $(0.05,10)$ in Figures 4 and 5, respectively. From Table 2, the relative error in the approximation of p/q is quite large in these cases and dramatically affects the coverage probabilities of the PR/SPR bounds. In general, the PR and SPR procedures are not suitable for large values of p, q (e.g., when $p, q > 0.001$).

The LR procedure doesn't depend on $(t_w/t_c)^\beta$ as an approximation of q/p, and its performance is less sensitive to changes in the value of this factor. Instead, the convergence of the LR coverage probabilities to the nominal confidence level depends mostly on Np. The LR approximate bounds proved to be adequate, and often excellent, in most of our numerical studies (usually when $Np \geq 10$).

Figures 3 to 5 fail to reveal if the coverage probabilities for the PR/SPR prediction bounds coverage asymptotically, as a function of Np, to any consistent limit. Large sample theory can explain the asymptotic convergence of the LR coverage probabilities to the nominal confidence level, for each value of p and q/p. But it is difficult to determine analytically if the coverage probabilities associated with PR and SPR procedures converge definitively (for any p and q), because of the discrete joint distribution of (X, Y). However,

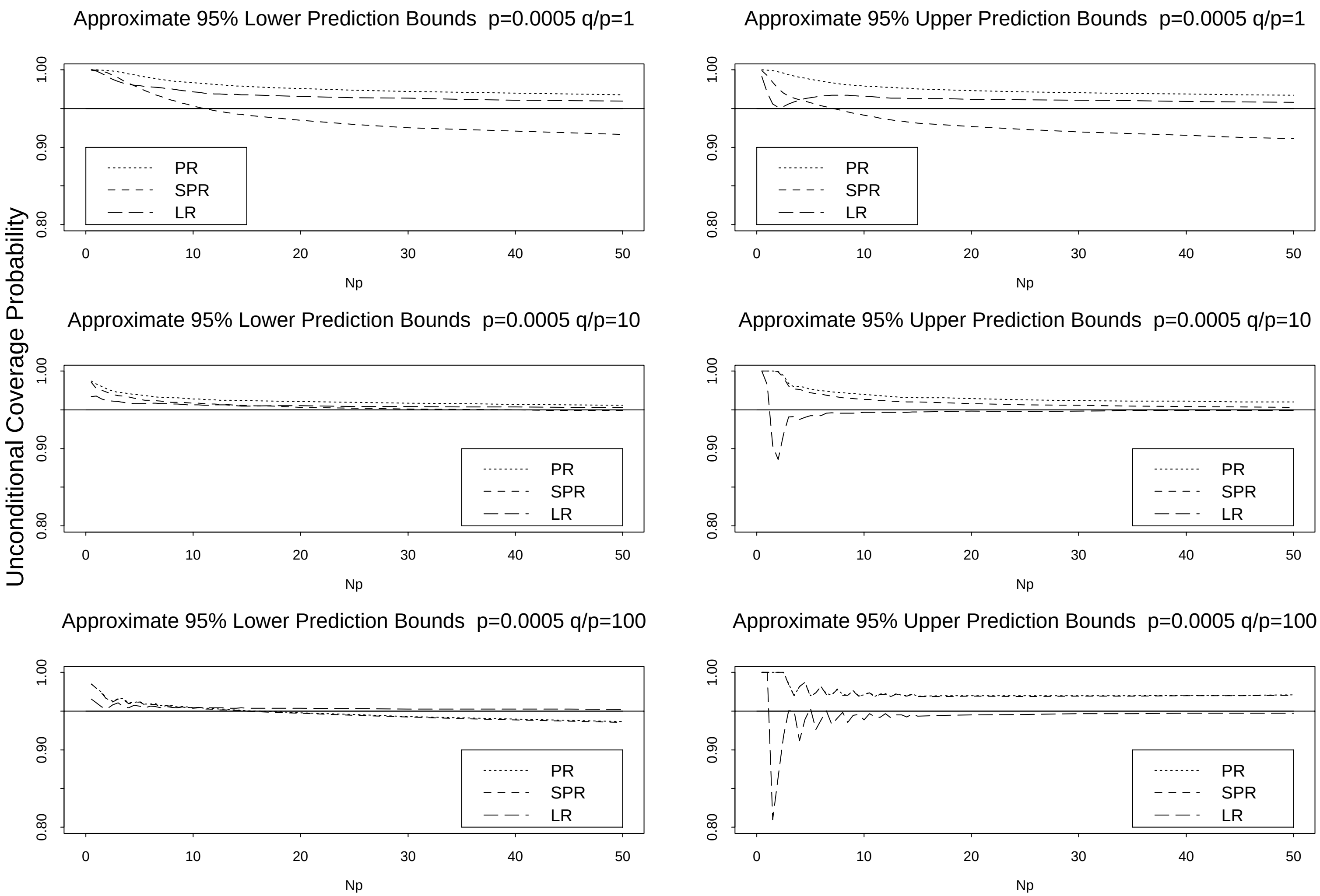

Figure 3: Plots of unconditional coverage probability versus expected number of failures (Np) for upper and lower one-sided approximate 95% prediction bounds from the probability ratio (PR), simplified probability ratio (SPR), and likelihood ratio (LR) procedures. $p = 0.0005$ and $q/p = 1$, 10, 100.

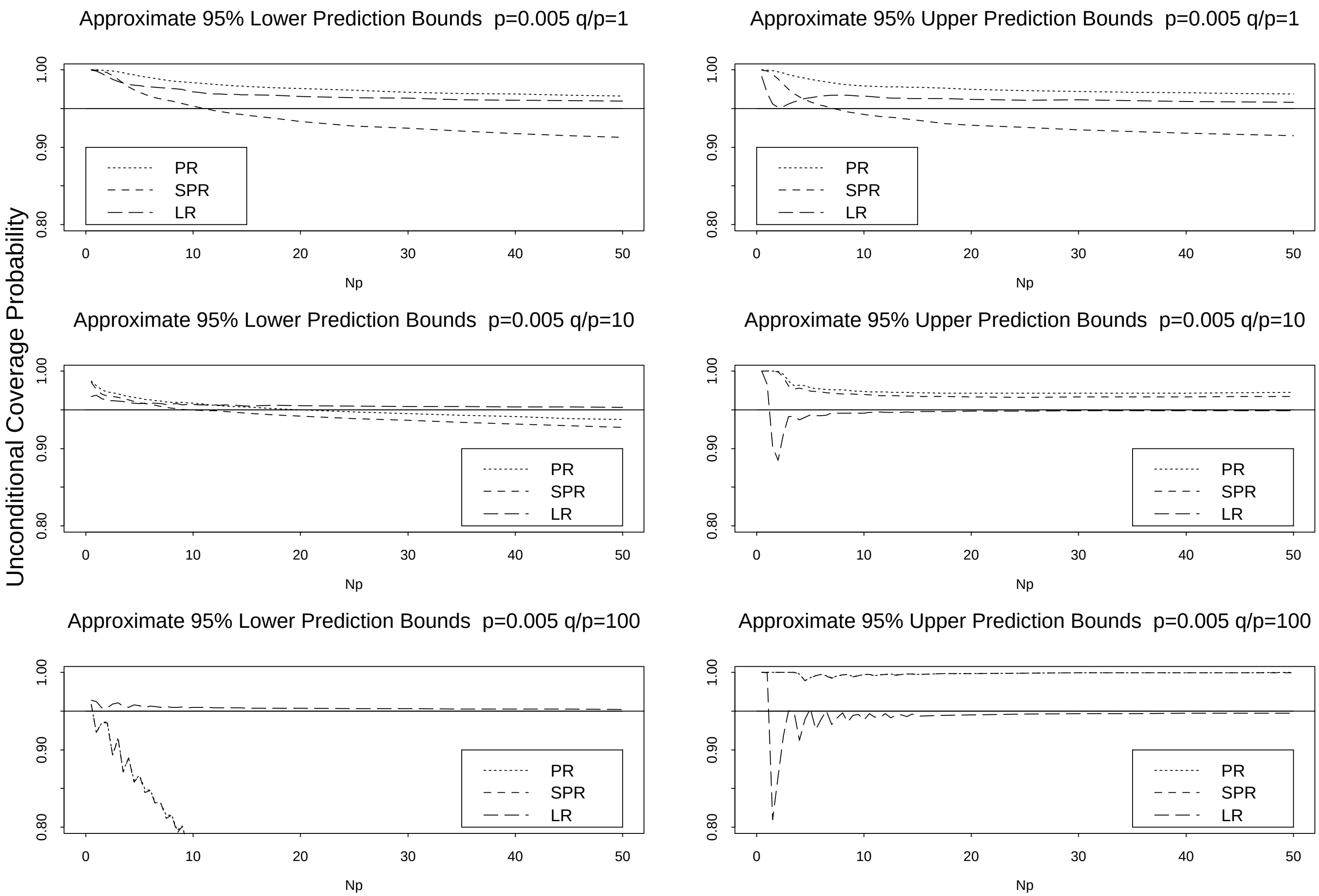

Figure 4: Plots of unconditional coverage probability versus expected number of failures (Np) for upper and lower one-sided approximate 95% prediction bounds from the probability ratio (PR), simplified probability ratio (SPR), and likelihood ratio (LR) procedures. $p = 0.005$ and $q/p = 1$, 10, 100.

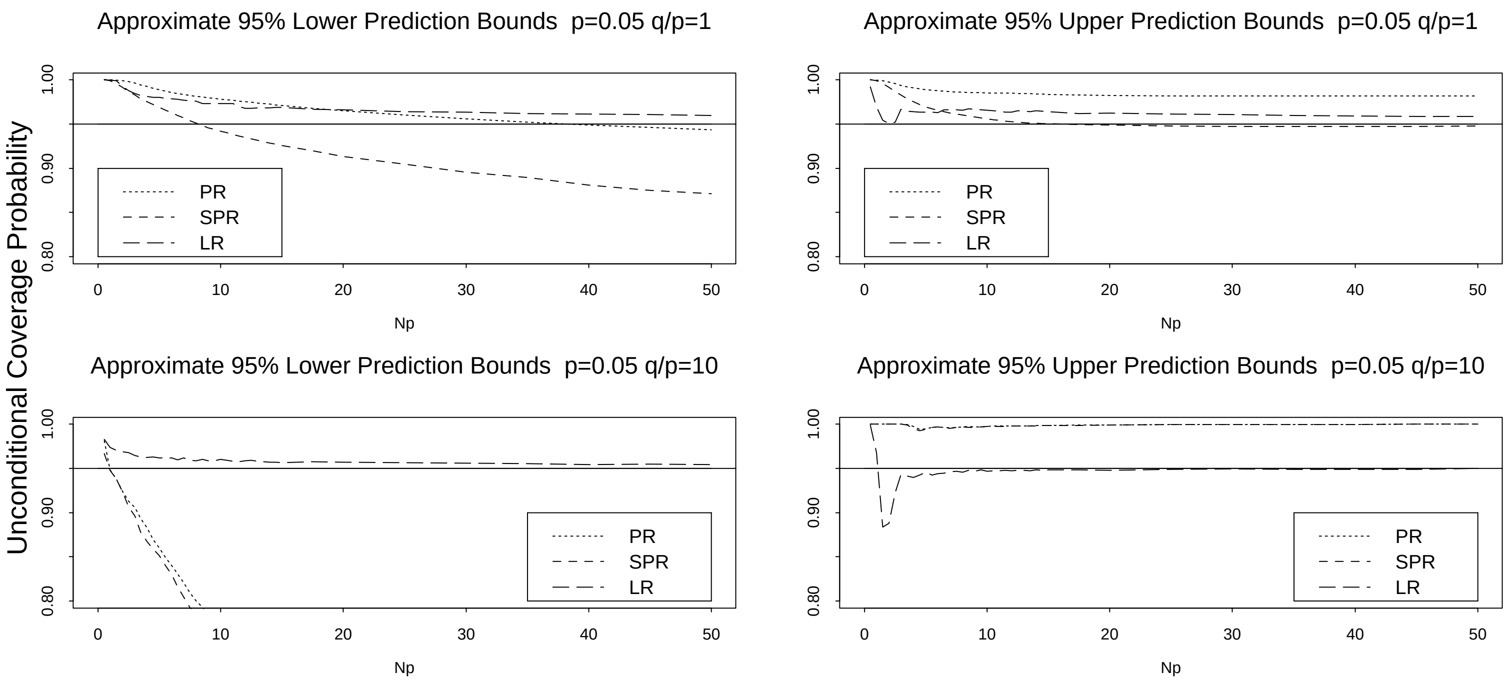

Figure 5: Plots of unconditional coverage probability versus expected number of failures (Np) for upper and lower one-sided approximate 95% prediction bounds from the probability ratio (PR), simplified probability ratio (SPR), and likelihood ratio (LR) procedures. $p = 0.05$ and $q/p = 1, 10$.

Table 3: Unconditional coverage probabilities of one-sided approximate 95% prediction bounds for several values of Np when $p = q = 0.1$. PR, SPR, and LR denote probability ratio, simplified probability ratio, and likelihood ratio procedures.

Np	Approx. 95% Lower Bounds			Approx. 95% Upper Bounds		
	PR	SPR	LR	PR	SPR	LR
5	0.96017	0.93452	0.97617	0.99283	0.98552	0.96019
10	0.93308	0.88983	0.96670	0.99142	0.98357	0.95795
15	0.90858	0.86376	0.96438	0.99230	0.98512	0.95779
20	0.88921	0.83151	0.96291	0.99294	0.98694	0.95623
30	0.84288	0.78431	0.95953	0.99487	0.98963	0.95537
50	0.78142	0.69469	0.95798	0.99707	0.99373	0.95511
100	0.62500	0.52271	0.95581	0.99913	0.99796	0.95343
300	0.22481	0.15487	0.95320	0.99998	0.99994	0.95205
500	0.06983	0.04114	0.95249	1.00000	1.00000	0.95162
750	0.01416	0.00707	0.95207	1.00000	1.00000	0.95137

other numerical studies have shown that, for $p, q > .01$, the PR and SPR LPBs have coverage probabilities that quickly converge to 0 as Np increases, while the coverage probabilities for the UPBs converge to 1. Table 3 illustrates this relationship between Np and the PR/SPR coverage probabilities when $p = q = 0.1$, listing coverage probabilities of one-sided approximate 95% UPBs and LPBs for each procedure.

8 Conclusions

The performance of the new prediction interval procedures may be characterized as follows:

- The LR procedure provides adequate approximate bounds with moderately large values of Np for any values of p and q. The associated coverage probabilities converge to the nominal confidence level as Np increases.

- The PR and SPR prediction interval procedures are appropriate only for small values of p and q [typically, small $(t_w/t_c)^\beta$]. For given p and q, the approximation does not improve with increasing Np.

- The performance of the PR and SPR procedures greatly depends on $(t_w/t_c)^\beta$ providing an adequate approximation for p/q; the accuracy of

LR procedure is not sensitive to the adequacy of this approximation.

The PR and SPR intervals are relatively easy to compute. In particular, the SPR bounds can be computed directly from chi-square quantiles. With modern computing, however, the LR prediction bounds are not too difficult to calculate and should be recommended when computing facilities can be used.

Acknowledgements

We would like to thank Wayne Nelson for suggesting that we work on this problem and for his detailed comments on an earlier version of this paper. A referee, the Associate Editor, and the Editor provide valuable comments that helped us to improve the paper. Computing for the research reported in this paper was done with equipment purchased with funds provided by a National Science Foundation SCREMS grant award DMS 9707740.

Appendix

Boundary properties of Nelson's (2000) prediction bounds

The approximate $100(1-\alpha_2)\%$ upper prediction bound from the probability ratio (PR) procedure in Section 4.2 is the "ceiling" of the real y such that

$$g_{\mathrm{U}}(y, X, \alpha_2) = \frac{1}{(t_w/t_c)^\beta - 1}. \tag{18}$$

An analogous statement holds for the PR lower prediction bound. For fixed X and $0 < \alpha < 1$, both $g_{\mathrm{U}}(y, X, \alpha)$ and $g_{\mathrm{L}}(y, X, \alpha)$ are decreasing functions of y such that $g_{\mathrm{U}}(y, X, \alpha) = O\left(X/y\right)$ and [assuming $X \neq 0$] $g_{\mathrm{L}}(y, X, \alpha) = O\left(X/y\right)$. When the number of failures X or the factor $(t_w/t_c)^\beta - 1$ is relatively large, it may be the case that $g_{\mathrm{U}}(N-X, X, \alpha_2) > 0$ or $g_{\mathrm{L}}(N-X, X, \alpha_1) > 0$. That is, the PR procedure may produce an upper prediction bound (and indeed even a lower bound) for the number of failures in (t_c, t_w) that is greater than $N-X$. An identical situation may arise with the simpler probability ratio-based bounds in (12), since they are derived from limiting forms of $g_{\mathrm{L}}(y, X, \alpha_1)$ and $g_{\mathrm{U}}(y, X, \alpha_2)$.

An intuitive explanation for the difficulties with the probability ratio-based procedures, in these extreme cases, follows. If X and Y are the numbers of failures in the intervals $(0, t_c]$ and (t_c, t_w) respectively, the maximum likelihood estimator for the ratio q/p is

$$\widehat{\rho} = Y/X.$$

If we knew the true value of q/p, we could obtain a simple prediction for the future realization of Y as

$$\dot{Y} = X \times q/p \tag{19}$$

by equating the probability ratio q/p to $\widehat{\rho}$. Equivalently, $\dot{Y}$ is simply the real-y such that

$$X/y - p/q = 0. \tag{20}$$

If N sample units are initially on trial, $\dot{Y}$ may potentially fall outside the sample space for sufficiently large X. As X approaches N, the prediction $\dot{Y}$ becomes increasingly larger, even though $Y \leq N - X$ with probability 1.

A prediction bound resulting from the probability ratio procedure behaves much like $\dot{Y}$. The PR prediction bound for Y is the real value at which a univariate function resembling X/y in form equals an approximation for p/q (18). As with $\dot{Y}$, a PR bound is less likely to fall outside the sample space of Y for sufficiently small $(t_w/t_c)^{\beta}$ (corresponding to a small ratio q/p).

For illustration, reconsider the heat exchanger example from Section 5 in which we wished to find prediction bounds for the additional number of exchanger tubes cracking (failing) in the span of $t_c = 3$ to $t_w = 10$ years. As before, we will use $N = 20{,}000$ and $\beta = 3.3$. When deriving an approximate lower 95% prediction bound for the added number of defective tubes, both $\underset{\sim}{Y}_{\mathrm{pr}}$ and $\underset{\sim}{Y}_{\mathrm{spr}}$ would be greater than $N - X$ for $X \geq 417$. As for an approximate upper 95% bound, both $\tilde{Y}_{\mathrm{pr}}$ and $\tilde{Y}_{\mathrm{spr}}$ would be greater than $N - X$ if $X \geq 351$.

An extreme prediction bound can also result from the likelihood ratio procedure. For (fixed) nonzero X, it can be shown that the log likelihood ratio test statistic $\mathcal{Q}(X, y)$ in (16), as a function of y, attains a minimum of zero at

$$\begin{aligned} y_{\min} &= N\left([1 - (X/N)] - [1 - (X/N)]^{(t_w/t_c)^{\beta}}\right) \\ &= \widehat{Y}, \end{aligned}$$

where $\widehat{Y}$ is from (6).

We also have that

$$\lim_{X \to N^-} \frac{[1-(X/N)]^{(t_w/t_c)^\beta}}{[1-(X/N)]} = 0.$$

Depending on $(t_w/t_c)^\beta$, the convergence of $[1-(X/N)]^{(t_w/t_c)^\beta}$ to zero may be rapid. Hence, for sufficiently large X, $N-X-1 < y_{\min} \le N-X$. This implies that the likelihood ratio-based upper prediction bound $\tilde{Y}_{\text{lr}}$ may be $N-X$ if X is large (as may be expected). Also, $\mathcal{Q}(X,y)$ tends to increase rapidly from its minimum at $y_{\min}$ with large X. In this case, the lower prediction bound produced by the likelihood ratio procedure will be close to $N-X$ and eventually equal $N-X-1$.

When using the likelihood ratio procedure to obtain an approximate upper 95% prediction bound for the future added number of cracked heat exchanger tubes with $N = 20{,}000$ and $\beta = 3.3$, $\tilde{Y}_{\text{lr}}$ would equal $N-X$ if $X \ge 2962$. The approximate lower 95% prediction bound $\underset{\sim}{Y}_{\text{lr}}$ for the added number of defective tubes would equal $N-X-1$ if $X \ge 3904$.

Likelihood ratio prediction bounds when $X = 0$

If there are no observed failures by t_c, it is possible that, for all real $y \in (0,\, N]$,

$$\mathcal{Q}(X=0, y) > \chi^2(1-\alpha; 1).$$

In this event, we let $\underset{\sim}{Y}_{\text{lr}} = 0$ and $\tilde{Y}_{\text{lr}} = N$. This cannot happen for nonzero X since $\mathcal{Q}(X \ne 0, y = y_{\min}) = 0$.

(Note also that $\mathcal{Q}(x=0, y=0)$ does not exist; when x and y equal zero, the constrained Weibull likelihood, $\mathcal{K}(x=0, y=0 \mid \eta) = \exp\left[-N(t_w/\eta)^\beta\right]$, does not have a maximum with respect to $\eta > 0$.)

Proof that $\left((t_w/t_c)^\beta - 1\right)^{-1}$ is less than p/q

Given probabilities $0 < p, q < 1$ from (1),

$$\frac{1}{(t_w/t_c)^\beta - 1} = \frac{1}{\frac{\log(1-p-q)}{\log(1-p)} - 1} = \frac{\log(1-p)}{\log(1-\frac{q}{1-p})} < \frac{p}{q} \Leftrightarrow \frac{q\log(1-p)}{p\log(1-\frac{q}{1-p})} < 1.$$

Fix $p \in (0,1)$. Then for $q \in (0, 1-p)$,

$$\frac{d}{dq}\left(\frac{q\log(1-p)}{p\log(1-\frac{q}{1-p})}\right) = \left(\frac{\log(1-p)}{p}\right)\left(\frac{\log(\frac{1-p-q}{1-p}) + \frac{1-p}{1-p-q} - 1}{\left[\log(1-\frac{q}{1-p})\right]^2}\right) < 0,$$

since $\log(x) + x^{-1} > 1$ for $x \in (0,1)^*$. The above function of q is decreasing.

For $q \in (0, 1-p)$,

$$\frac{q\log(1-p)}{p\log(1-\frac{q}{1-p})} \leq \lim_{q\to 0+} \frac{q\log(1-p)}{p\log(1-\frac{q}{1-p})} = \log(1-p)\left(1-\frac{1}{p}\right) < 1,$$

using $-(1-x)\log(1-x) < x$ for $x \in (0,1)^{**}$.

* and ** can be shown with a first order Taylor expansion of $\log(x)+x^{-1}$ around 1 and $-(1-x)\log(1-x)$ around 0. □

Thus,

$$\frac{q\log(1-p)}{p\log(1-\frac{q}{1-p})} < 1$$

for all values of p, q from (1), implying that approximation $\left((t_w/t_c)^\beta - 1\right)^{-1}$ is always less than the true probability ratio p/q.

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