Analysis and comparison of Bayesian methods for type A uncertainty evaluation with prior knowledge

Ignacio Lira

Prolegomenon

Data : $\{x_1, x_2, \ldots, x_n\}$

GUM: estimate $x = \frac{1}{n}\sum_{i=1}^{n} x_i$

standard uncertainty $u_{\texttt{GUM}} = \left(\frac{s^2}{n}\right)^{1/2}$;

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x - x_i)^2$$

▹ formula is based on frequentist concepts

GUM-S1: standard uncertainty $u_{\texttt{GUM-S1}} = \phi \times u_{\texttt{GUM}}$;

$$\phi = \sqrt{\frac{n-1}{n-3}}$$

▹ formula derived from the Bayesian paradigm

- assuming a Gaussian likelihood
- using no prior knowledge about nei-

ther μ nor v

▹ Problem: evaluating ϕ requires at least four

observations

Proposals - 1

Informative Bayesian Type A uncertainty evaluation for a small number of observations

Cox and Shirono, Metrologia 54 (2017)

Appears to be the first paper that proposes solving the problem by taking advantage of knowledge that may be available before measurements.

Its authors applied Bayes' formula to a Gaussian likelihood and an informative prior proportional to $1/v$ for $v_{\mathtt{min}} \leq v \leq v_{\mathtt{max}}$

Using some clever manipulations, they were able to derive an analytic expression for factor ϕ involving the upper incomplete gamma function.

Result can be easily obtained with the Wolfram Mathematica© software

In[1]:=

```
Example 4.3 in C - S;

n = 2;
x = {0.9551, 0.9537};
mean = Mean[x];
s = StandardDeviation[x];
sM = 0.003;
sm = 0.001;
```

$S = (n - 1)\, s^2;$

$as = \frac{n-3}{2};\; ai = \frac{n-1}{2};$

$a = \frac{S}{2\, sM^2};\; b = \frac{S}{2\, sm^2};$

$phi = \left(\frac{n-1}{2}\,\frac{Gamma[as, a] - Gamma[as, b]}{Gamma[ai, a] - Gamma[ai, b]}\right)^{1/2};$

$uGum = \frac{s}{\sqrt{n}};$

```
uCS = phi uGum;
Print["uCS      = " , uCS]
Print["uGum     = " , uGum]
```

```
uGum     = 0.0007
uCS      = 0.0012686
```

Alternatively, one can use direct numerical application of Bayes theorem

In[16]:=
```
Example 4.3 in C - S using mumerical integration;  (13 s);

p0[mu_, v_] := If[sm^2 ≤ v ≤ sM^2, 1/v, 0]
l[mu_, v_] := 1/v^(n/2) Exp[-(S + n (mu - mean)^2)/(2 v)]
p1[mu_, v_] := p0[mu, v] × l[mu, v]
p2[mu_] := NIntegrate[p1[mu, v], {v, sm^2, sM^2}]
c = (Quiet[NIntegrate[p2[mu], {mu, -∞, ∞}]])^-1;
expec = Quiet[NIntegrate[mu c p2[mu], {mu, -∞, ∞}]];
stdev =
  (Quiet[NIntegrate[(mu - expec)^2 c p2[mu], {mu, -∞, ∞}]])^(1/2);
unum = stdev;
Print["unum  = " , unum]
Print["uCS   = " , uCS]
```

```
uCS   = 0.0012686
unum  = 0.00126859
```

The method in the C-S paper requires $n \geq 2$.
But the numerical procedure applies even for one observation e.g.

```
In[27]:= x = 0.9551; (13 s);
p0[mu_, v_] := If[sm^2 ≤ v ≤ sM^2, 1/v, 0]
l[mu_, v_] := 1/v^(1/2) Exp[-(mu - x)^2/(2 v)]
p1[mu_, v_] := p0[mu, v] × l[mu, v]
p2[mu_] := NIntegrate[p1[mu, v], {v, sm^2, sM^2}]
c = (Quiet[NIntegrate[p2[mu], {mu, -∞, ∞}]])^-1;
expec = Quiet[NIntegrate[mu c p2[mu], {mu, -∞, ∞}]];
stdev =
  (Quiet[NIntegrate[(mu - expec)^2 c p2[mu], {mu, -∞, ∞}]])^(1/2);
Print["u 1 obs = ", stdev]
Print["u 2 obs = ", uCS]
u 2 obs = 0.0012686
u 1 obs = 0.00190813
```

Proposals - 2

Bayesian methods for type A evaluation of standard uncertainty
van der Veen, Metrologia 55 (2018)

In this paper, its author proposes using a half-Cauchy prior for the standard deviation, that is, a *t*-Student with one dof. I will write such a prior in the form $p(\mu, v) \propto (A+v)^{-1}$.

The median of this distribution can be made equal to an available prior estimate of the variance. In this way, a reasonable value for the parameter A can be obtained.

The resulting posterior does not have a closed form. Of course, it can be evaluated through MCMC, as the paper cited above does. But as the following example demonstrates, it is simpler (and faster) to use the numerical procedure just described.

In[37]:=

```
Example 4.3 using a half – Cauchy prior;

x = {0.9551, 0.9537};  (24 s);
```

$$m = \left(\frac{sM\ sm}{sM + sm}\right)^2;$$

$$A = \frac{m}{-1 + \sqrt{e}};$$

$$p0[mu\_, v\_] := (A + v)^{-1}$$

$$l[mu\_, v\_] := \frac{1}{v^{n/2}} \operatorname{Exp}\left[-\frac{S + n\ (mu - mean)^2}{2\ v}\right]$$

```
p1[mu_, v_] := p0[mu, v] × l[mu, v]
p2[mu_] := NIntegrate[p1[mu, v], {v, 0, ∞}]
```

$$c = (Quiet[NIntegrate[p2[mu], \{mu, -\infty, \infty\}]])^{-1};$$

```
expec = Quiet[NIntegrate[mu c p2[mu], {mu, -∞, ∞}]];
stdev =
```

$$\left(Quiet\left[NIntegrate\left[(mu - expec)^2\ c\ p2[mu], \{mu, -\infty, \infty\}\right]\right]\right)^{1/2};$$

```
uCauchy = stdev;
Print["uCauchy = ", uCauchy]
Print["uCS     = ", uCS]

uCS     = 0.0012686
uCauchy = 0.531866
```

Proposals - 3

A simple method for Bayesian uncertainty evaluation in linear models
Wübbeler, Marschall and Elster, Metrologia 57 (2020)

This paper applies to measurement models of the form $Y = \alpha X + B$, where B represents a linear combination of type B quantities. But by taking $B = 0$ (and $\alpha = 1$), we recover our measurement model.

The authors assume an inverse gamma prior for the variance of the sampling distribution of repeated measurements of X. If in addition we ignore previous knowledge about the value of the measurand, we are left with

$$p(\mu, v) \propto \left(\frac{1}{v}\right)^{1+a} \exp\left(-\frac{b}{v}\right)$$

The authors suggest $a = 1$, which produces a weakly informative prior with neither finite mean nor variance. With this choice, the median of the distribution, equal to $b/\ln 2$, can again be taken as the prior estimate of the variance, if available. In this way the value of parameter b is obtained.

In[51]:=

```
Example 4.3 using an inverse gamma prior;  (11 s);

x = {0.9551, 0.9537};
a = 1;
m = (sM sm)/(sM + sm);
b = m Log[2];
p0[mu_, v_] := 1/v^(1+a) Exp[-b/v]
l[mu_, v_] := 1/v^(n/2) Exp[-(S + n (mu - mean)^2)/(2 v)]
p1[mu_, v_] := p0[mu, v] × l[mu, v]
p2[mu_] := NIntegrate[p1[mu, v], {v, 0, ∞}]
c = (Quiet[NIntegrate[p2[mu], {mu, -∞, ∞}]])^-1;
expec = Quiet[NIntegrate[mu c p2[mu], {mu, -∞, ∞}]];
stdev =
  (Quiet[NIntegrate[(mu - expec)^2 c p2[mu], {mu, -∞, ∞}]])^(1/2);
ugamma = stdev;
Print["ugamma   = ", ugamma]
Print["uCauchy  = ", uCauchy]
Print["uCS      = ", uCS]
```

```
uCS      = 0.0012686
uCauchy  = 0.531866
ugamma   = 0.0228108
```

However, the inverse gamma prior produces a marginal posterior for the measurand equal to a scaled and shifted t-distribution , whose variance can be calculated as

$$\frac{2b+(n-1)s^2}{n(n+2a-3)}$$

Verification:

In[67]:=
```
Print[Sqrt[(2 b + (n - 1) s^2)/(n (n + 2 a - 3))]]
Print[ugamma]
```
```
0.0228108
0.0228112
```

From this formula we see that the inverse gamma prior can again be used if there is only one observation, but in that case the shape parameter a has to be greater that 1.

Proposals - 4 (last)

An informed type A evaluation of standard uncertainty valid for any sample size greater than or equal to 1
Carobbi, Acta Imeko 11 (2022)

This paper, which seems to be the most recent contributor to this discussion, proposes using a scaled inverse chi-square distribution as an informative prior:

$$p(\mu, v) \propto \left(\frac{1}{v}\right)^{1+\nu/2} \exp\left(-\frac{\sigma_0^2\,\nu}{2v}\right)$$

where σ_0^2 is the prior variance and ν is the associated number of degrees of freedom. Clearly, this distribution describes the same data structure as the inverse gamma, but with a different parameterization, the relation between the two parameters being
$\nu = 2a$ and $\sigma_0^2 = \frac{b}{a}$.

In[69]:=

```
Example 4.3 using a scaled inverse chi - square distribution; (14 s);

x = {0.9551, 0.9537};
nu = 2 a;
s02 = b/a;
p0[mu_, v_] := 1/v^(1+nu/2) Exp[- (s02 nu)/(2 v)]
l[mu_, v_] := 1/v^(n/2) Exp[- (S + n (mu - mean)^2)/(2 v)]
p1[mu_, v_] := p0[mu, v] × l[mu, v]
p2[mu_] := NIntegrate[p1[mu, v], {v, 0, ∞}]
c = (Quiet[NIntegrate[p2[mu], {mu, -∞, ∞}]])^-1;
expec = Quiet[NIntegrate[mu c p2[mu], {mu, -∞, ∞}]];
stdev =
  (Quiet[NIntegrate[(mu - expec)^2 c p2[mu], {mu, -∞, ∞}]])^(1/2);
Print["ugamma   = ", ugamma]
Print["uchi2    = ", stdev]
```

```
uchi2    = 0.0228108
ugamma   = 0.0228108
```

So, mathematically, it doesn't matter whether one uses the inverse γ or the inverse χ^2 prior. However, the proposal by Carobbi is more intuitive, because as Gelman *et*. *al*. point out in their famous book, the scaled inverse χ^2 can be thought of as providing the information equivalent to ν observations with average squared deviation σ_0^2. These two parameters may be available from prior experiments.

Closure

So, what conclusions can we draw from this exposition?

1) The Cox-Shirono approach produces comparatively very small uncertainties. This appears to be the result of a strongly informative prior. Perhaps another form of the function $p(\mu, v)$ supported on the interval $[v_{\mathtt{min}}, v_{\mathtt{max}}]$ might produce more reasonable results.

2) This comment elicits a query: would there be a way of quantifying the "informativeness" of a prior?

3) For generality, I wrote the prior as $p(\mu, v)$, even though in none of the proposals it depends on μ. That is to say, I have assumed that there is absolutely no prior information on the value of the measurand. Evidently, this assumption simplifies matters, but it is not very reasonable. A better approach is the one used by Wübbeler *et*. *al*. , who propose a NIG prior.

4) If one decides to keep with the assumption of constant μ, the inverse γ and inverse χ^2 priors produce a simple algebraic formula for the standard uncertainty, usable by all practitioners. However the latter prior may be preferred because its parameters have an intuitive interpretation.

5) In simple cases, the Mathematica software allows direct numerical exploration of other priors, such as plotting the marginal posteriors or computing credible intervals, without the need to use MCMC or other alternatives.

See also

Guidance on Bayesian uncertainty evaluation for a class of GUM measurement models   Demeyer, Fischer and Elster , Metrologia 58 (2021)

Simple informative prior distributions for metrology
O’Hagan and Cox, Unpublished (2021)

Uncertainty evaluations from small datasets
Stoud, Pintar and Possolo, Metrologia 58 (2021)

Rejection sampling for Bayesian Uncertainty evaluation using the Monte Carlo techniques of GUM-S1
Marschall, Wübbeler and Elster , Metrologia 59 (2022)

For a pdf copy of this presentation please send an email to
ilira@ing.puc.l