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Bayesian uncertainty analysis under prior ignorance of the measurand versus analysis using the Supplement 1 to the *Guide*: a comparison

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Abstract
A recent supplement to the GUM (GUM S1) is compared with a Bayesian analysis in terms of a particular task of data analysis, one where no prior knowledge of the measurand is presumed. For the Bayesian analysis, an improper prior density on the measurand is employed. It is shown that both approaches yield the same results when the measurand depends linearly on the input quantities, but generally different results otherwise. This difference is shown to be not a conceptual one, but due to the fact that the two methods correspond to Bayesian analysis under different parametrizations, with ignorance of the measurand expressed by a non-informative prior on a different parameter. The use of the improper prior for the measurand itself may result in an improper posterior probability density function (PDF) when the measurand depends non-linearly on the input quantities. On the other hand, the PDF of the measurand derived by the GUM supplement method is always proper but may sometimes have undesirable properties such as non-existence of moments.

It is concluded that for a linear model both analyses can safely be applied. For a non-linear model, the GUM supplement approach may be preferred over a Bayesian analysis using a constant prior on the measurand. But since in this case the GUM S1 PDF may also have undesirable properties, and as often some prior knowledge about the measurand may be established, metrologists are strongly encouraged to express this prior knowledge in terms of a proper PDF which can then be included in a Bayesian analysis. The results of this paper are illustrated by an example of a simple non-linear model.

1. Introduction

In a recent supplement to the GUM [1], evaluation of measurement uncertainty is proposed in terms of a probability density function (PDF) which expresses the knowledge about the value of the measurand. This supplement [2]—hereafter called GUM S1—starts from a model which relates the measurand to a number of input quantities. Having specified the (joint) PDF on the input quantities, GUM S1 describes how to numerically determine the resulting PDF of the measurand.

GUM S1 also specifies how to assign a PDF for the input quantities in various cases. When independent observations of an input quantity from an assumed Gaussian distribution are given, a shifted and scaled t-distribution is assigned to that quantity. It was shown in [3] that in these instances the PDF resulting from an application of GUM S1 can also be derived by a Bayesian analysis using Bayes' theorem, provided that particular non-informative priors are chosen.

When both data and prior knowledge of the measurand are available, a Bayesian analysis most conveniently starts from an observation equation rather than from the model employed by the GUM [4]. In that case the prior knowledge about the measurand is accounted for in the construction of the prior density. Such Bayesian solution differs from that of GUM S1 as the presence of prior knowledge of the measurand is not directly considered in GUM S1. While the Bayesian approach is generally applicable once the prior and the sampling distribution of the data have been specified, GUM S1 gives guidance on the assignment of PDFs for the input quantities only for particular sampling distributions.

GUM S1 describes how to determine numerically the PDF for the measurand that is—due to the model relation—uniquely determined by a transformation of variables from the PDFs of the input quantities. If in this situation additional *independent* knowledge of the measurand is available in terms of a PDF, reference [5] proposes a method of merging these two densities. In particular, the PDF derived by GUM S1 and the additional PDF are multiplied and the result is normalized to produce a PDF. This can be numerically done by a simple modification of the Monte Carlo method of GUM S1, cf [5].

As has been pointed out in [6], GUM S1 can yield different results in the analysis of data than a Bayesian analysis starting from an observation equation, even in the case of Gaussian observations and no prior information about the measurand. In this paper we take a closer look at this observation. We do this for a particular but generic situation of data analysis in metrology for which GUM S1 is applicable. After presenting the results of both approaches, we rewrite the GUM S1 solution in terms of a Bayesian analysis. This allows the differences in the assumptions underlying both treatments to be identified. We show that the results may differ due to the (implicit) choice of priors. It turns out that the same PDFs are obtained when the measurand depends linearly on the input quantities and when a constant prior for the measurand is utilized in the Bayesian analysis. Thus, in general both approaches will be equivalent in the absence of prior knowledge (when expressed by a constant improper prior for the Bayesian approach) only for linear models; otherwise, different results will be obtained. We critically assess the considered choices of non-informative priors in the absence of prior knowledge. We argue that a constant, improper prior on the measurand itself in a Bayesian analysis appears to be inappropriate when the measurand depends non-linearly on the input quantities. We illustrate the implications by a non-linear example. We show that for the chosen example, a Bayesian analysis which uses a constant improper prior yields an improper posterior PDF in contrast to the GUM S1 solution. We then compare the results with those obtained by a Bayesian analysis when prior knowledge on the measurand can be utilized. Finally, we close by drawing some conclusions of these findings.

2. Task of data analysis

Let Y denote the measurand, and

$$Y = f(X, Z) \tag{1}$$

the model relation in terms of the GUM [1]. X and Z serve as a 'type A' and 'type B' variable, respectively, that is, there are data points from which X can be estimated but none for Z. In order to keep the notation simple, we consider only one input variable of each type. To illustrate such a situation, consider a simple version of example H1 of [1]. This concerns a measurement of length of a nominally (at 20 °C) 50 mm end gauge. We can define Y to be the length of the gauge at 20 °C, X to be the length of the gauge at the actual temperature (for example 25 °C) and Z to be $(1+\alpha\theta)$ where α is the coefficient of thermal expansion and θ is the deviation in temperature from 20 °C.

The model (1) is assumed to be uniquely solvable for X according to

$$X = g(Y, Z). \tag{2}$$

Under the Bayesian approach, the unknown value of a quantity is modelled by a random variable whose density represents the available knowledge about it. We use upper case letters to denote random variables and lower case letters for possible values of them. The PDF of a random variable X is denoted by $p(x)$, and the joint PDF of random variables X and Y by $p(x, y)$ or—where required—by $p_{(X,Y)}(x, y)$.

The available information about the input quantities is as follows. A proper PDF $p(z)$ represents our knowledge about Z. In the simple example, this is based on knowledge of the coefficient of thermal expansion and of the deviation in temperature from 20 °C. We further assume that the observations $d_1, \ldots, d_n$ are independent realizations from a Gaussian density with expectation X and variance Σ^2. No prior knowledge about X, Y and Σ is at hand.

3. Bayesian analysis

For the Bayesian analysis we consider the parametrization

$$\boldsymbol{\theta} = (Y, Z, \Sigma). \tag{3}$$

The posterior PDF $p(\boldsymbol{\theta}|d_1, \ldots, d_n)$ is obtained via Bayes' theorem as

$$p(\boldsymbol{\theta}|d_1, \ldots, d_n) \propto p(\boldsymbol{\theta}) l(\boldsymbol{\theta}|d_1, \ldots, d_n), \tag{4}$$

where $p(\boldsymbol{\theta})$ denotes the prior density on $\boldsymbol{\theta}$ and the likelihood function $l(\boldsymbol{\theta}|d_1, \ldots, d_n)$ is given by

$$l(\boldsymbol{\theta}|d_1, \ldots, d_n) = \prod_{i=1}^{n} \frac{\mathrm{e}^{-(d_i - g(y,z))^2/2\sigma^2}}{\sqrt{2\pi\sigma^2}}. \tag{5}$$

Prior densities summarize knowledge available about a quantity before any updating via Bayes' theorem is performed. To distinguish the prior density for Y from other densities for the measurand considered in this paper, we denote it by $p_0(y)$. We consider the three parameters to be *a priori* independent and so $p(\boldsymbol{\theta}) = p_0(y)p(z)p(\sigma)$. Since no knowledge about Σ is available, and since it acts as a scale parameter in the likelihood (5), we will use the standard non-informative prior $p(\sigma) \propto 1/\sigma$ [7]. Thus,

$$p(\boldsymbol{\theta}) = p(y, z, \sigma) \propto p_0(y)p(z)/\sigma. \tag{6}$$

As y plays neither the role of a location nor that of a scale parameter in (5), no ready-made non-informative prior is available. We will first derive the posterior density of the measurand using the common improper non-informative prior density $p_0(y) \propto 1$. In our simple example, this prior density expresses the fact that we are ignorant of the length of the gauge at 20 °C. In section 5 we return to the issue of choice of non-informative prior density for Y.

After some simplification, (4) yields

$$\begin{aligned} p(y|d_1, \ldots, d_n) &\propto \int p(y, z, \sigma) l(y, z, \sigma | d_1, \ldots, d_n)\, \mathrm{d}\sigma\, \mathrm{d}z \qquad (7) \\ &\propto p_0(y) \int p(z) \frac{t_{n-1}[(g(y,z) - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}}\, \mathrm{d}z \end{aligned}$$

for the posterior PDF for the measurand. Here $\bar{d}$ and s denote mean and standard deviation of the observations $d_1, \ldots, d_n$, and $t_{n-1}[\cdot]$ the PDF of a t-distributed random variable with $n-1$ degrees of freedom. Integrating the posterior PDF of Y for $p_0(y) \propto 1$ by applying change-of-variable we obtain

$$\int p(y|d_1, \ldots, d_n)\, \mathrm{d}y \propto \int\int \frac{1}{|\partial g/\partial y|} p(z) \frac{t_{n-1}[(x - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}}\, \mathrm{d}z\, \mathrm{d}x, \qquad (8)$$

where $\partial g/\partial y$ is evaluated at $(f(x,z), z)$. Thus, under the assumption of $p_0(y) \propto 1$, the Bayesian posterior of the measurand is clearly a proper density (integrates to 1) when $g(y, z)$ is linear since then

$$\int p(y|d_1, \ldots, d_n)\, \mathrm{d}y \propto \int\int p(z) \frac{t_{n-1}[(x - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}}\, \mathrm{d}z\, \mathrm{d}x = 1 \qquad (9)$$

holds. But the right-hand side of (8) may not be bounded in general. Thus, the usual non-informative density $p_0(y) \propto 1$ cannot be applied routinely.

4. GUM S1

For our particular problem, GUM S1 assigns the scaled and shifted t-distribution,

$$p(x) = \frac{t_{n-1}[(x - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}}, \qquad (10)$$

to X. Then, assuming independence between the random variables X and Z, their joint PDF is

$$p(x, z) = \frac{t_{n-1}[(x - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} p(z). \qquad (11)$$

To obtain the PDF $p(y)$ for the measurand Y from $p(x, z)$, the model relation (1) is employed to first derive from (11) the joint PDF $p(y, z)$ by application of the *change-of-variables formula*, leading to

$$p(y, z) = |\partial g/\partial y| \frac{t_{n-1}[(g(y,z) - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} p(z), \qquad (12)$$

where $|\partial g/\partial y|$ denotes the determinant of the Jacobian entering the transformation formula and is evaluated at (y, z). Subsequent marginalization with respect to z then yields

$$p(y) = \int |\partial g/\partial y| \frac{t_{n-1}[(g(y,z) - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} p(z)\, \mathrm{d}z. \qquad (13)$$

The PDF (13) differs from the Bayesian posterior density (7) by the prior $p_0(y)$ in (7) and by the term $|\partial g/\partial y|$ in (13), but this implies that when no prior knowledge about the measurand is available, and the Bayesian approach is employed with $p_0(y) \propto 1$, both approaches yield the same results when the model (1) is linear. Otherwise, different PDFs are obtained in general. It is of interest to check whether $p(y)$ is a proper density. We get

$$\begin{aligned} \int p(y)\, \mathrm{d}y &= \int\int |\partial g/\partial y| \frac{t_{n-1}[(g(y,z) - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} p(z)\, \mathrm{d}z\, \mathrm{d}y \\ &= \int p(z)\, \mathrm{d}z = 1. \qquad (14) \end{aligned}$$

The PDF $p(y)$ (13) can also be derived as a Bayesian posterior under the parametrization $\widetilde{\Theta} = (X, Z, \Sigma)$ instead of $\Theta = (Y, Z, \Sigma)$. Such a parametrization is—in principle—of equal value since due to relations (1) and (2) there is a one-to-one correspondence between Θ and $\widetilde{\Theta}$. Assuming independence among the three parameters and taking $p(x) \propto 1$, we obtain

$$p(\tilde{\theta}) = p(x, z, \sigma) = p(x)p(z)p(\sigma) \propto p(z)/\sigma. \qquad (15)$$

It is useful to recall the simple example, and note that here the ignorance being expressed by $p(x)$ is of the length of the gauge at the actual measurement temperature, rather than at 20 °C. The likelihood (5) in terms of $\widetilde{\Theta}$ is

$$l(\tilde{\theta}|d_1, \ldots, d_n) = \prod_{i=1}^{n} \frac{\mathrm{e}^{-(d_i - x)^2/2\sigma^2}}{\sqrt{2\pi\sigma^2}}. \qquad (16)$$

Application of Bayes' theorem and subsequent marginalization with respect to σ immediately yields

$$\begin{aligned} p_{(X,Z)}(x, z|d_1, \ldots, d_n) &\propto \int p(\tilde{\theta}) l(\tilde{\theta}|d_1, \ldots, d_n)\, \mathrm{d}\sigma \qquad (17) \\ &\propto \frac{t_{n-1}[(x - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} p(z). \end{aligned}$$

The right-hand side of (17) equals the PDF in (11), from which in the same way as above the PDF (13) is derived for the posterior $p(y|d_1, \ldots, d_n)$. Thus the GUM S1 PDF (13) results from a Bayesian analysis using the parametrization $\widetilde{\Theta} = (X, Z, \Sigma)$ and the particular improper priors $p(x) \propto 1$ and $p(\sigma) \propto 1/\sigma$.

While both parametrizations $\Theta = (Y, Z, \Sigma)$ and $\widetilde{\Theta} = (X, Z, \Sigma)$ are valid, only the former allows for a simple incorporation of available prior knowledge about the measurand Y. On the other hand, the use of the usual improper prior ($p(x) \propto 1$) to denote ignorance in the parametrization $\widetilde{\Theta} = (X, Z, \Sigma)$ leads to a proper density for Y for any proper density for Z. This is not the case for the parametrization $\Theta = (Y, Z, \Sigma)$ and the improper prior $p_0(y) \propto 1$.

5. Discussion

GUM S1 and the Bayesian analysis yield the same results when the model relation (1) is linear and the Bayesian analysis employs the improper prior $p_0(y) \propto 1$. Otherwise, different results will emerge in general. Since the PDF derived by GUM S1 may also be derived from an application of Bayes' theorem, the difference between the approaches is not conceptual but is due to different parametrizations and different priors. This type of difference in PDFs derived under different parametrizations with improper priors has been observed in other applications and has been referred to as the *marginalization paradox* [8, 9]. Whether this truly represents a paradox or not is a matter of opinion with [9] representing the view that it does not.

The question of how to express ignorance of the measurand is clearly important. In Bayesian analysis, when no prior knowledge about a parameter is available, non-informative (usually, improper) priors are utilized. However, the construction of such priors is not straightforward, there is no unique density that represents ignorance. For a sampling distribution of the data d of the form $p(d|\eta, \upsilon) \propto h[(d-\eta)/\upsilon]/\upsilon$, the function $p(\eta, \upsilon) \propto 1/\upsilon$ is viewed as a standard non-informative prior [7] for the location and scale parameters η and υ. In our data analysis problem, the pair (y, σ) are not location and scale parameters when the model is non-linear, cf the likelihood (5), and it was shown above that $p(y, \sigma) \propto 1/\sigma$ may lead to an improper posterior for Y. For the parametrization $\widetilde{\Theta} = (X, Z, \Sigma)$ on the other hand, (x, σ) is a pair of a location and scale parameter, cf the likelihood (16), and hence the prior $p(x, z, \sigma) \propto p(z)/\sigma$ is the usual non-informative prior and leads to a proper posterior for Y. Note, however, that this prior expresses ignorance of X and not of Y.

Different concepts such as probability matching priors [10] or reference priors [11] have been proposed for assigning non-informative priors. While the former concept attempts to determine the prior such that the posterior will ensure exact or approximate frequentist coverage properties of credibility regions, the latter seeks a prior for which the gain in information of the posterior relative to the prior is in some sense maximized. It turns out that for the multivariate case the reference prior may depend on the final single parameter of interest; i.e. different multivariate reference priors on $(\eta_1, \ldots, \eta_p)$ may be obtained depending on which η_i is the parameter of interest and which are the nuisance parameters. It may be interesting to see what an approximate probability matching prior or a reference prior would look like for this example, but this is beyond the scope of this paper.

In the case of informative prior knowledge on the measurand Y the parametrization $\boldsymbol{\Theta} = (Y, Z, \Sigma)$ is to be preferred, and the PDF (7)—with $p_0(y)$ expressing the prior knowledge about the measurand—should be used instead of GUM S1.

The modification of GUM S1 proposed in [5] to account for prior knowledge about the measurand may also be considered. The same results would be obtained when the model relation (1) is linear, and different results otherwise. However, as mentioned in the introduction, the approach [5] aims at merging (independent) information. It should be used when GUM S1 is applied for fully specified PDFs on the input quantities rather than for the task of data analysis considered here. The reason is that in the former case redundant information on the measurand (i.e. a prior PDF and the PDF derived by GUM S1) is available and needs to be merged. In the case of data analysis considered in this paper, such merging would be of an informative prior on the measurand and a Bayesian posterior obtained in using the particular *improper* prior underlying GUM S1. It is not sensible to perform a Bayesian analysis with a non-informative prior when in fact information is available. Therefore, a Bayesian analysis using Bayes' theorem together with the prior information on the measurand is to be preferred in such a case. But note that when in addition also prior knowledge on X would be available (i.e. X would be a mixture of a 'type A and type B variable'), some redundant information would be given and should be merged. But this situation is not considered in GUM S1.

6. Example

Consider the example

$$Y = f(X, Z) = X/Z, \tag{18}$$

$$X = g(Y, Z) = Y \cdot Z. \tag{19}$$

The PDF on Z is assumed to be

$$p(z) = \begin{cases} 1 & z \in (0, 1], \\ 0 & \text{otherwise}. \end{cases} \tag{20}$$

In this case, GUM S1 and the Bayesian analysis yield

$$p(y) = \int_0^1 z \frac{t_{n-1}[(y \cdot z - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} \, \mathrm{d}z, \tag{21}$$

and

$$p(y|d_1, \ldots, d_n) \propto p_0(y) \int_0^1 \frac{t_{n-1}[(y \cdot z) - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} \, \mathrm{d}z, \tag{22}$$

respectively.

Consider first the case when no prior knowledge on the measurand is available. Figure 1 shows the resulting GUM S1 PDF (21) for $n = 8$ observations $d_1, \ldots, d_8$ on X with mean $\bar{d} = 1$ and standard deviation $s = 1$. As we noted previously, the density $p(y)$ (21) integrates to one. However, the first and all higher moments do not exist for this PDF, and hence the expectation as the usual estimate cannot be determined here. Nonetheless, credibility intervals on the measurand could be established. The PDF (22) obtained by the Bayesian approach when using the prior $p_0(y) \propto 1$ on the other hand is improper, since

$$\int_{-\infty}^{\infty} \left(\int_0^1 \frac{t_{n-1}[(y \cdot z) - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}} \, \mathrm{d}z \right) \mathrm{d}y = \int_0^1 \frac{1}{z} \, \mathrm{d}z = \infty, \tag{23}$$

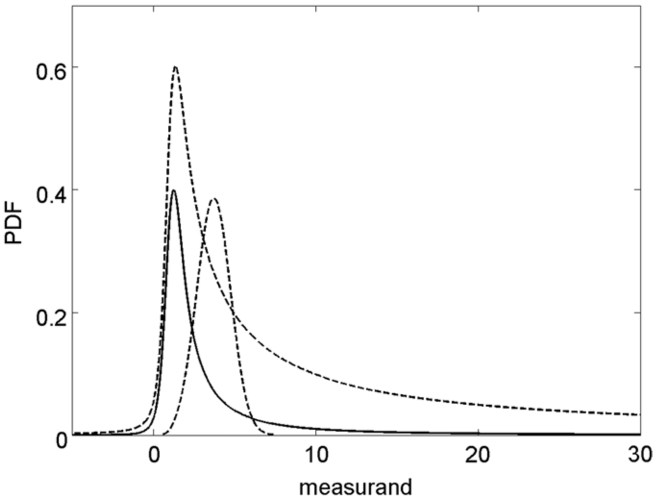

Figure 1. Results for the considered example: GUM S1 PDF (solid line) and improper Bayesian posterior (dashed line, large tail) in the absence of prior knowledge on the measurand. In addition, the Bayesian posterior is shown (dashed line, small tail) when prior knowledge on the measurand is utilized.

and yields no solution here. A common substitute prior density for $p_0(y) \propto 1$ is a Gaussian density with a large variance. We have examined the behaviour of the Bayesian solution under such an alternative prior for Y. It produces a proper posterior density for Y, one which has all moments, but the moments and highest probability density intervals are quite sensitive to the size of the prior variance. Thus it is not a satisfactory alternative prior density in this problem. There is one feature of the densities of Y that is rather robust to the choice of prior, however, and that is the mode. We were able to show that the posterior mode of Y under the Gaussian prior becomes the posterior mode under the improper prior as the variance approaches infinity. Further, figure 1 shows that the modes of the GUM S1 PDF and the improper Bayes posterior are quite close.

In this particular example, the lack of moments for the GUM S1 density of Y and the impropriety of the Bayesian posterior density are due to the fact that the density $p(z)$ allows values arbitrarily close to zero. For the Bayesian solution in particular, note that expression (8) results for this example with a density $p(z)$ in a proper posterior density for Y if

$$\int \frac{1}{|z|} p(z)\, \mathrm{d}z < \infty. \tag{24}$$

Thus, more information on Z (whose value should be non-zero) could imply a sufficient decay of the PDF which would then produce a proper posterior density for Y. In this sense, the problems of the posterior density of Y are due not just to having no information about Y itself but in addition, also to having only 'vague' (insufficient) information on Z.

To illustrate how informative prior information about the measurand affects the results, assume next that the Gaussian density with mean equal to 4 and variance equal to 1 describes the available prior knowledge about Y. When this particular density is employed in (22), a proper posterior is obtained. This is illustrated by figure 1. The resulting estimate and its associated standard uncertainty are obtained as $y = 3.7$ and $u(y) = 1.0$. Note that all higher moments of this PDF exist.

7. Conclusions

Application of GUM S1 to the analysis of data can be viewed as a Bayesian analysis using a particular improper prior. Differences in the resulting densities of the GUM S1 and a Bayesian analysis starting from an observation equation have been identified as due to the different parametrizations and priors underlying both analyses. When the model between the measurand and the input quantities is linear and the Bayesian analysis employs a constant improper prior on the measurand, the two methods yield the same results. Otherwise, different results are obtained in general.

For a non-linear model, a constant improper prior on the measurand is not expected to be uniformly appropriate for a Bayesian analysis in the absence of prior knowledge. Other non-informative priors such as reference priors may be considered. When prior knowledge about the measurand is available, metrologists are encouraged to express it in a proper prior density on the measurand which can then be included in the Bayesian analysis.

The relatively simple data analysis problem considered here illustrates an important fact applicable to many more complex cases. This is that examination and careful consideration of all of the PDFs used in either approach are extremely important.

Appendix

We briefly outline the derivation of equation (7). By inserting (5) and (6) into (4) we obtain

$$\begin{aligned} &p(y, z, \sigma | d_1, \ldots, d_n) \\ &\quad \propto p_0(y)p(z)/\sigma \cdot \prod_{i=1}^{n} \frac{\mathrm{e}^{-(d_i - g(y,z))^2/2\sigma^2}}{\sqrt{2\pi\sigma^2}} \\ &\quad \propto p_0(y)p(z)\frac{1}{\sigma^{n+1}}\mathrm{e}^{-[n(g(y,z)-\bar{d})^2+(n-1)s^2]/2\sigma^2}, \end{aligned} \tag{A1}$$

where $\bar{d}$ and s denote mean and standard deviation of the observations $d_1, \ldots, d_n$. Marginalization of (A1) with respect to σ yields

$$\begin{aligned} &p(y, z | d_1, \ldots, d_n) \\ &\quad \propto p_0(y)p(z)\int_0^\infty \frac{1}{\sigma^{n+1}}\mathrm{e}^{-[n(g(y,z)-\bar{d})^2+(n-1)s^2]/2\sigma^2}\,\mathrm{d}\sigma \\ &\quad \propto p_0(y)p(z)\left(1 + \frac{[(g(y,z)) - \bar{d})/(s/n^{1/2})]^2}{n-1}\right)^{-n/2} \\ &\quad \propto p_0(y)p(z)\frac{t_{n-1}[(g(y,z) - \bar{d})/(s/n^{1/2})]}{s/n^{1/2}}. \end{aligned} \tag{A2}$$

By finally marginalizing (A2) with respect to z (7) is obtained.

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