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Computation of Signal–to–Noise Ratios

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Abstract: Using elementary results from the statistics literature, the exact distributions are derived for the experimental signal–to–noise ratio (SNR) and its variants. These distributions together with well established computer programs can be used to derive various properties (e.g. critical values) of quotients of experimental SNRs.

1 Introduction

The experimental signal–to–noise ratio (SNR) and its variants play a pivotal role in analytical chemistry and related areas. Often, in the chemistry literature, tables of critical values of quotients of experimental SNRs are obtained by Monte Carlo simulation, see e.g. Voigtman (1997). We feel that this is unnecessary because, as explained below, a better treatment could be provided by what is known in the statistics literature.

2 Exact Distributions of SNRs

Suppose $x_1, x_2, \ldots, x_N$ is a random sample from a Gaussian population with mean μ and standard deviation σ. The true SNR is μ/σ and the experimental SNR is defined as

$$\mathrm{SNR} = \frac{\bar{x}}{s} \tag{1}$$

(see equation (1) in Voigtman (1997)), where $\bar{x}$ is the sample mean defined by

$$\bar{x} = \frac{x_1 + x_2 + \cdots + x_N}{N} \tag{2}$$

and s is the sample standard deviation defined by

$$s = \sqrt{\frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N - 1}}. \tag{3}$$

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Consider also the following variations of (1):

$$\mathrm{SNR}' = \frac{\bar{x}}{s'} \tag{4}$$

and

$$\mathrm{SNR}_e = \frac{\bar{x}}{s_e} \tag{5}$$

as well as the relative standard deviation defined by

$$\mathrm{RSD} = \frac{s}{\bar{x}}, \tag{6}$$

where $s' = s\sqrt{(N-1)/N}$ and $s_e = s/\sqrt{N}$. Finally, consider the quotients of SNRs defined by

$$\mathrm{R} = \frac{\bar{x}_2/s_2}{\bar{x}_1/s_1}, \tag{7}$$

$$\mathrm{R}_e = \mathrm{R}\sqrt{\frac{\nu_2+1}{\nu_1+1}} \tag{8}$$

and

$$\mathrm{R}_r = \frac{1}{\mathrm{R}} \tag{9}$$

(see equations (13)–(15) in Voigtman (1997)), where $(\bar{x}_1, \bar{x}_2)$ are the sample means and (s_1, s_2) are the sample standard deviations for two independent random samples of size (ν_1+1, ν_2+1) from a Gaussian population with mean μ and standard deviation σ.

The probability distributions of the quantities defined in (1)–(9) can be determined by elementary results in mathematical statistics. Using the sampling theory for the Gaussian distribution, one can determine that $\bar{x}$ has the Gaussian distribution with mean μ and standard deviation $\sigma/\sqrt{N}$ independently of s. We write

$$\bar{x} \sim N\left(\mu, \frac{\sigma}{\sqrt{N}}\right), \tag{10}$$

where "$\sim$" has the meaning "has the same distribution as." Using the fact that

$$\sum_{i=1}^{N} (x_i - \bar{x})^2 \sim \sigma^2 \chi^2_{N-1},$$

where χ^2_ν denotes the well–known chi–square distribution with degrees of freedom ν, one see that

$$\begin{aligned} s &\sim \sqrt{\frac{\sigma^2 \chi^2_{N-1}}{N-1}} \\ &\sim \frac{\sigma \chi_{N-1}}{\sqrt{N-1}}, \end{aligned} \tag{11}$$

$$\begin{aligned} s' &\sim \frac{\sqrt{N-1}s}{\sqrt{N}} \\ &\sim \frac{\sigma \chi_{N-1}}{\sqrt{N}}, \end{aligned} \tag{12}$$

and

$$\begin{aligned} s_e &\sim \frac{s}{\sqrt{N}} \\ &\sim \frac{\sigma \chi_{N-1}}{\sqrt{N(N-1)}}. \end{aligned} \tag{13}$$

The exact distributions of the SNRs given by (1) and (4)–(6) can be determined by using the definition of the non–central t distribution. If X is a Gaussian random variable with mean δ and unit standard deviation and $Y \sim \chi^2_\nu$ is independent of X then

$$T = \frac{X}{\sqrt{Y/\nu}} \quad \sim \quad t_{\nu,\delta} \tag{14}$$

is said to have the well–known non–central t distribution with degrees of freedom ν and non–centrality parameter δ. The probability density function (pdf) of T is given by

$$f_T(t) \quad = \quad \frac{\exp\left(-\delta^2/2\right)\Gamma\left((1+\nu)/2\right)}{\sqrt{\pi\nu}\Gamma\left(\nu/2\right)} \left(\frac{\nu}{\nu+t^2}\right)^{(1+\nu)/2} \sum_{j=0}^{\infty} \frac{\Gamma\left((1+\nu+j)/2\right)}{j!\Gamma\left((1+\nu)/2\right)} \left(\frac{t\delta\sqrt{2}}{\sqrt{\nu+t^2}}\right)^j \tag{15}$$

for $t > 0$ (see Johnson *et al.* (1995)). Using (10)–(13) and (14), one can determine that

$$\begin{aligned} \mathrm{SNR} &\sim \frac{N\left(\mu, \sigma/\sqrt{N}\right)}{(\sigma/\sqrt{N-1})\chi_{N-1}} \\ &\sim \frac{(\sigma/\sqrt{N})N\left((\sqrt{N}/\sigma)\mu, 1\right)}{(\sigma/\sqrt{N-1})\chi_{N-1}} \\ &\sim \frac{1}{\sqrt{N}} \frac{N\left((\sqrt{N}/\sigma)\mu, 1\right)}{(1/\sqrt{N-1})\chi_{N-1}} \\ &\sim \frac{1}{\sqrt{N}} t_{N-1,\sqrt{N}\mu/\sigma}, \end{aligned} \tag{16}$$

$$\begin{aligned} \mathrm{SNR}' &\sim \frac{N\left(\mu, \sigma/\sqrt{N}\right)}{(\sigma/\sqrt{N})\chi_{N-1}} \\ &\sim \frac{(\sigma/\sqrt{N})N\left((\sqrt{N}/\sigma)\mu, 1\right)}{(\sigma/\sqrt{N})\chi_{N-1}} \\ &\sim \frac{1}{\sqrt{N-1}} \frac{N\left((\sqrt{N}/\sigma)\mu, 1\right)}{(1/\sqrt{N-1})\chi_{N-1}} \\ &\sim \frac{1}{\sqrt{N-1}} t_{N-1,\sqrt{N}\mu/\sigma}, \end{aligned} \tag{17}$$

$$\mathrm{SNR}_e \sim \frac{N\left(\mu, \sigma/\sqrt{N}\right)}{(\sigma/\sqrt{N(N-1)})\chi_{N-1}}$$

$$
\begin{aligned}
&\sim \frac{(\sigma/\sqrt{N})N\left((\sqrt{N}/\sigma)\mu, 1\right)}{(\sigma/\sqrt{N(N-1)})\chi_{N-1}} \\
&\sim \frac{N\left((\sqrt{N}/\sigma)\mu, 1\right)}{(1/\sqrt{N-1})\chi_{N-1}} \\
&\sim t_{N-1,\sqrt{N}\mu/\sigma}, \qquad (18)
\end{aligned}
$$

and

$$
1/\mathrm{RSD} \sim \frac{1}{\sqrt{N}} t_{N-1,\sqrt{N}\mu/\sigma}. \qquad (19)
$$

The corresponding pdfs can be expressed in the form of $f_T(\cdot)$ given by (15). The pdfs of SNR, SNR$'$, SNR$_e$ and RSD are $\sqrt{N} f_T(\sqrt{N}t)$, $\sqrt{N-1} f_T(\sqrt{N-1}t)$, $f_T(t)$ and $(\sqrt{N}/t^2) f_T(\sqrt{N}/t)$, respectively, with $\nu = N - 1$ and $\delta = \sqrt{N}\mu/\sigma$.

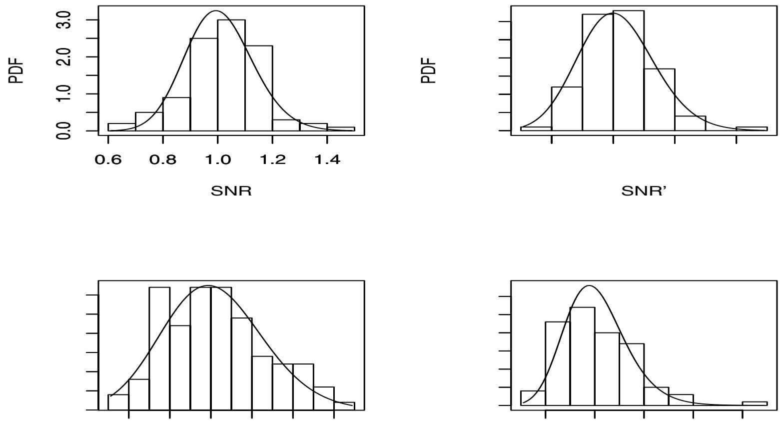

Figure 1. Histograms of simulated data on SNR, SNR$'$, SNR$_e$ and RSD superimposed with the exact pdfs given by (16)–(19). We have chosen $\mu = 1$, $\sigma = 1$ and $N = 100$.

We now provide a graphical illustration of the *exactness* of the results in (16)–(19). We simulated 100 samples of $x_1, x_2, \ldots, x_N$ each with $\mu = 1$, $\sigma = 1$ and $N = 100$. For each sample, we computed $\bar{x}$ and s and hence SNR, SNR$'$, SNR$_e$ and RSD. So, we end up with 100 values of SNR, 100 values of SNR$'$, 100 values of SNR$_e$ and 100 values of RSD. Then, we compared the histograms of these 100 values with the corresponding exact pdfs, i.e. compare the histogram for SNR with $\sqrt{N} f_T(\sqrt{N}t)$, the histogram for SNR$'$ with $\sqrt{N-1} f_T(\sqrt{N-1}t)$, the histogram for SNR$_e$ with $f_T(t)$ and the histogram for RSD with $(\sqrt{N}/t^2) f_T(\sqrt{N}/t)$. The results are shown in Figure 1. Clearly, the non–central t distribution describes the data remarkably well. The non–central t distribution arises also in other areas of chemistry. See Malcolm (1984) and Li *et al.* (2001).

Finally, consider the quotients of SNRs defined by (7)–(9). It follows immediately from (16)–(19)

that

$$\mathrm{R} \sim \sqrt{\frac{\nu_1+1}{\nu_2+1}} \frac{t_{\nu_2,\sqrt{\nu_2+1}\mu/\sigma}}{t_{\nu_1,\sqrt{\nu_1+1}\mu/\sigma}},$$

$$\mathrm{R}_e \sim \frac{t_{\nu_2,\sqrt{\nu_2+1}\mu/\sigma}}{t_{\nu_1,\sqrt{\nu_1+1}\mu/\sigma}},$$

and

$$1/\mathrm{R}_r \sim \sqrt{\frac{\nu_1+1}{\nu_2+1}} \frac{t_{\nu_2,\sqrt{\nu_2+1}\mu/\sigma}}{t_{\nu_1,\sqrt{\nu_1+1}\mu/\sigma}}.$$

The corresponding pdfs require the study of the ratio of non–central t random variables. Suppose $X \sim t_{a_1,\delta_1}$ and $Y \sim t_{a_2,\delta_2}$ are independent non–central t random variables and let $Z = X/Y$. Using (15), the pdf of Z can be written as

$$\begin{aligned}
f_Z(z) &= \int_0^\infty t f_X(t) f_Y(zt) dt \\
&= \frac{a_1^{a_1/2} a_2^{a_2/2} \exp\left(-\delta_1^2/2 - \delta_2^2/2\right)}{\pi\Gamma\left(a_1/2\right)\Gamma\left(a_2/2\right)} \\
&\quad \times \int_0^\infty \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{\Gamma\left((1+a_1+j)/2\right)\Gamma\left((1+a_2+k)/2\right)\left(\delta_1\sqrt{2}\right)^j\left(\delta_2\sqrt{2}\right)^k t^{j+k+1}}{j!k!\left(a_1+t^2\right)^{j+(a_1+1)/2}\left(a_2+z^2t^2\right)^{k+(a_2+1)/2}} dt \\
&= \frac{a_1^{a_1/2} a_2^{a_2/2} \exp\left(-\delta_1^2/2 - \delta_2^2/2\right)}{\pi\Gamma\left(a_1/2\right)\Gamma\left(a_2/2\right)} \\
&\quad \times \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{\Gamma\left((1+a_1+j)/2\right)\Gamma\left((1+a_2+k)/2\right)\left(\delta_1\sqrt{2}\right)^j\left(\delta_2\sqrt{2}\right)^k}{j!k!} \\
&\quad \times \int_0^\infty \frac{t^{j+k+1}}{\left(a_1+t^2\right)^{j+(a_1+1)/2}\left(a_2+z^2t^2\right)^{k+(a_2+1)/2}} dt \\
&= \frac{a_1^{a_1/2} a_2^{a_2/2} \exp\left(-\delta_1^2/2 - \delta_2^2/2\right)}{2\pi\Gamma\left(a_1/2\right)\Gamma\left(a_2/2\right)} \\
&\quad \times \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{\Gamma\left((1+a_1+j)/2\right)\Gamma\left((1+a_2+k)/2\right)\left(\delta_1\sqrt{2}\right)^j\left(\delta_2\sqrt{2}\right)^k}{j!k!} \\
&\quad \times \int_0^\infty \frac{w^{(j+k)/2}}{\left(a_1+w\right)^{j+(a_1+1)/2}\left(a_2+z^2w\right)^{k+(a_2+1)/2}} dw \\
&= \frac{a_1^{a_1/2} a_2^{a_2/2} \exp\left(-\delta_1^2/2 - \delta_2^2/2\right)}{2\pi\Gamma\left(a_1/2\right)\Gamma\left(a_2/2\right)} \\
&\quad \times \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{\Gamma\left((1+a_1+j)/2\right)\Gamma\left((1+a_2+k)/2\right)\left(\delta_1\sqrt{2}\right)^j\left(\delta_2\sqrt{2}\right)^k}{j!k!} I(j,k). \qquad (20)
\end{aligned}$$

By equation (2.2.6.24) in Prudnikov *et al.* (1986), the integral $I(j,k)$ can be calculated as

$$I(j,k) = a_1^{(1-j+k-a_1)/2} a_2^{-k-(a_2+1)/2} B\left(1+\frac{j+k}{2}, \frac{j+k+a_1+a_2}{2}\right)$$

$$\times {}_2F_1\left(1+\frac{j+k}{2}, k+\frac{a_2+1}{2}; j+k+1+\frac{a_1+a_2}{2}; 1-\frac{a_1 z^2}{a_2}\right),$$

where

$$B(a,b) = \int_0^1 w^{a-1}(1-w)^{b-1} dw$$

is the beta function and

$${}_2F_1\left(a,b;c;x\right) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{x^k}{k!},$$

is the Gauss hypergeometric function, where $(z)_k = z(z+1)\cdots(z+k-1)$ denotes the ascending factorial. Using the result in (20), the pdfs of R, R_e and $1/\mathrm{R}_r$ can be expressed as $\sqrt{(\nu_2+1)/(\nu_1+1)}$ $f_Z(\sqrt{(\nu_2+1)/(\nu_1+1)}z)$, $f_Z(z)$ and $(1/z^2)\sqrt{(\nu_2+1)/(\nu_1+1)}$ $f_Z(\sqrt{(\nu_2+1)/(\nu_1+1)}(1/z))$, respectively, with $a_1 = \nu_2$, $a_2 = \nu_1$, $\delta_1 = \sqrt{\nu_2 + 1}\mu/\sigma$ and $\delta_2 = \sqrt{\nu_1+1}\mu/\sigma$.

3 Conclusions

We have derived the exact distributions of the SNRs and their quotients (equations (1) and (4)–(9)) by using the established properties of the non–central t distribution. The *exactness* of the distributions has been verified by simulation. The non–central t distributions have been known since the early 1900s and their properties have been studied extensively in the statistics literature. The reader is referred to Chapter 31 of Johnson *et al* (1995) for the most up–to–date details on the distributions. Computer programs for evaluating the non–central t distributions are also widely available (e.g. in R, a freely downloadable statistical software) and these programs can be used to produce e.g. accurate tables of critical values without the need for Monte Carlo simulation.

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