The optimal division between sample and background measurement times

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I. SCOPE

Herein outlined is the method and calculation to determine how best to divide measurement time between a sample and the background, in order to minimize the relative uncertainty. Especially in the case of a Bonse-Hart camera, the measurement time division for each point can be optimized depending on the signal-to-noise ratio.

II. BACKGROUND

Usually, equal time is given to measuring the background and the sample, or even a longer background measurement is taken as it has so few counts. While this seems correct intuitively, the relative error after background subtraction improves when more time is spent counting the measurement with the highest amount of scattering. As there is usually limited time available on a SAXS machine, a good division must be found between measuring the background and sample, so that the uncertainty of the background-subtracted intensity is as low as possible.

III. THE CALCULATION - SAM'S WAY

We assume that the number of background intensity photons I_b, measured for a time t_b is subtracted from the sample measurement photon count I_s which was measured for a time t_s, to result in the background subtracted count rate C_{bs}:

$$C_{bs} = \frac{I_s}{t_s} - \frac{I_b}{t_b} \tag{1}$$

Defining the sample uncertainty as $\Delta I_s = \sqrt{I_s}$ and the background uncertainty similarly as $\Delta I_b = \sqrt{I_b}$, the uncertainty ΔC_{bs} would then be:

$$\Delta C_{bs} = \sqrt{\left(\frac{\Delta I_s}{t_s}\right)^2 + \left(\frac{\Delta I_b}{t_b}\right)^2} = \sqrt{\frac{I_s}{t_s^2} + \frac{I_b}{t_b^2}} \tag{2}$$

The uncertainty normalized to the intensity then becomes:

$$\frac{\Delta C_{bs}}{C_{bs}} = \frac{\sqrt{\frac{I_s}{t_s^2} + \frac{I_b}{t_b^2}}}{\frac{I_s}{t_s} - \frac{I_b}{t_b}} = \sqrt{\frac{\frac{I_s}{t_s^2} + \frac{I_b}{t_b^2}}{\left(\frac{I_s}{t_s} - \frac{I_b}{t_b}\right)^2}} = \sqrt{\frac{\frac{C_s}{t_s} + \frac{C_b}{t_b}}{(C_s - C_b)^2}} \tag{3}$$

Defining the number of counted photons I to be a multiplication of the count rate C and the measurement time, we get $I_b = C_b t_b$ and $I_s = C_s t_s$. Further defining the signal-to-noise ratio $g = \frac{C_s}{C_b}$, the total time $t_t = t_b + t_s$ and the fraction of time spent measuring the sample $f = \frac{t_s}{t_t}$, we can define our relative uncertainty in terms of signal-to-noise ratio and time fraction:

$$\frac{\Delta C_{bs}}{C_{bs}} = \sqrt{\frac{1}{C_b}}\sqrt{\frac{\frac{g}{t_s}+\frac{1}{t_b}}{(g-1)^2}} = \sqrt{\frac{1}{C_b}}\sqrt{\frac{\frac{g}{ft_t}+\frac{1}{(1-f)t_t}}{(g-1)^2}} = \sqrt{\frac{1}{C_b t_t}}\sqrt{\frac{\frac{g}{f}+\frac{1}{(1-f)}}{(g-1)^2}} \tag{4}$$

We then can try to find the optimum by locating the value for f where the derivative of equation 4 is zero:

$$\frac{\partial\frac{\Delta C_{bs}}{C_{bs}}}{\partial f} = \frac{\partial}{\partial f}\sqrt{\frac{1}{C_b t_t}}\sqrt{\frac{\frac{g}{f}+\frac{1}{(1-f)}}{(g-1)^2}} = 0 \tag{5}$$

$$0 = \frac{\partial}{\partial f}\sqrt{\frac{\frac{g}{f}+\frac{1}{(1-f)}}{(g-1)^2}} \tag{6}$$

which according to Wolfram Alpha:

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Solve[Assuming[g>0,D[sqrt((g/f+1/(1-f))/(g-1)^2),f]]=0,f]
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is true for

$$f = \frac{g \pm \sqrt{g}}{g-1} \tag{7}$$

Since f can only lie within $0 < f < 1$, only

$$f = \frac{g - \sqrt{g}}{g-1} \tag{8}$$

can be a solution.

We can calculate the relative reduction in uncertainty compared to the 50/50 case (i.e. equal time spent on background and sample measurements) as:

$$\frac{\frac{\Delta C_{bs}}{C_{bs}}\ |_{50/50} - \frac{\Delta C_{bs}}{C_{bs}}\ |_{\text{optimal}}}{\frac{\Delta C_{bs}}{C_{bs}}\ |_{50/50}} = \frac{\sqrt{\frac{2g+2}{(g-1)^2}} - \sqrt{\frac{\frac{g^2-g}{g-\sqrt{g}}+\frac{g-1}{\sqrt{g}-1}}{(g-1)^2}}}{\sqrt{\frac{2g+2}{(g-1)^2}}} \tag{9}$$

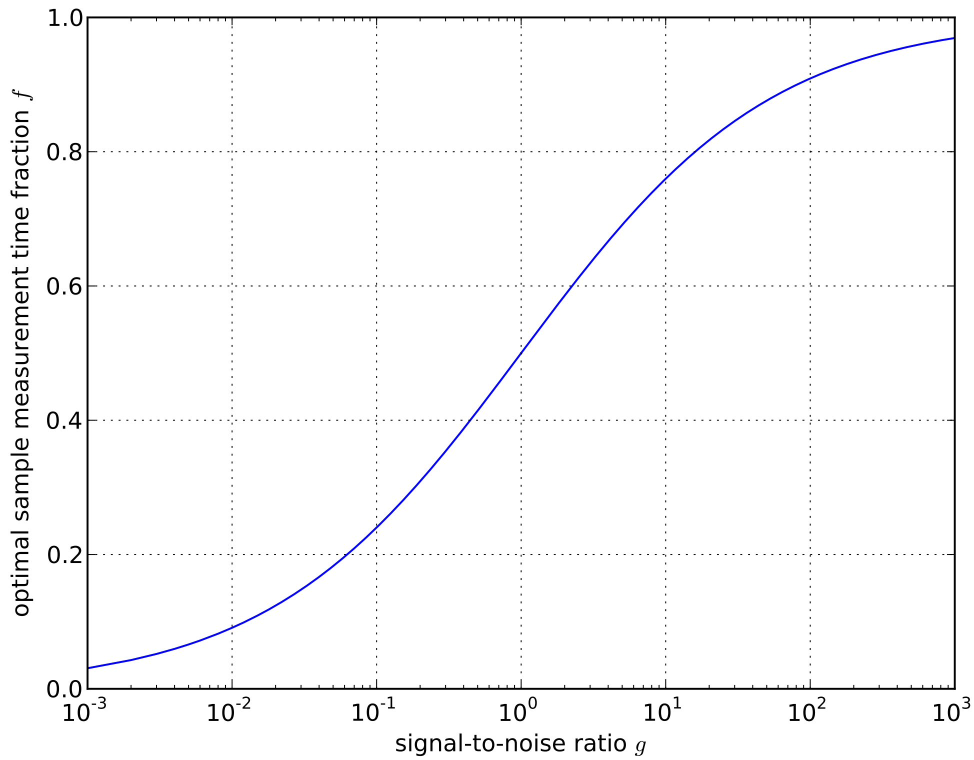

Figure 1. The optimal fraction of time f spent measuring the sample as opposed to measuring the background, as a function of the signal-to-noise ratio g.

IV. CONCLUSIONS

Figures 1 and 2 show the optimal division of time between sample and background, and the reduction in uncertainty obtained through this optimization. It can be shown that especially in areas of high differences in count rate between the sample and the background, the reduction in uncertainty may be worth the trouble of a quick determination of the signal-to-noise ratio.

Especially in the case of a Bonse-Hart camera, where the measurement time *per point* can be freely tuned, a quick scan of sample and background may be used to automatically select the most optimal use of measurement time.

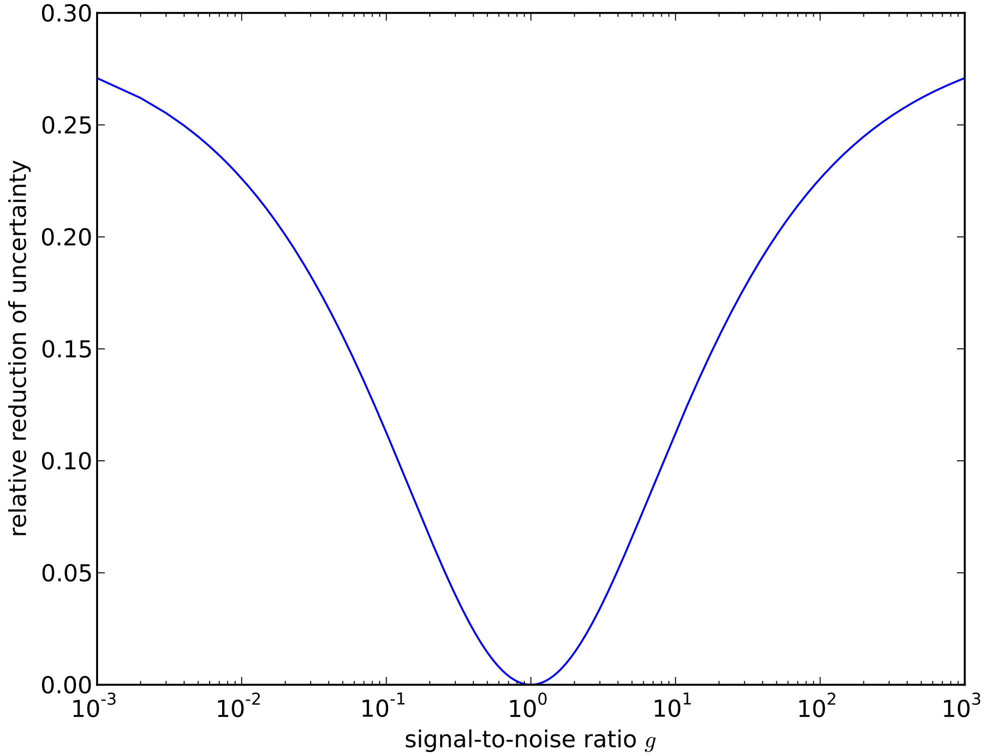

Figure 2. The reduction in error that can be obtained by dividing the time optimally between sample and background measurement, as a function of the signal-to-noise ratio g.