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Comment on Article by Hogg et al.

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The authors are to be congratulated for a well writing introduction to the analysis of Small Angle Neutron Scattering (SANS) experiments datasets. These experiments provide a powerful tool to explore the ferromagnetic properties of thin films and nanoparticles. The presented modeling framework for joint calibration data and experimental data is timely. It represents a paradigm shift from current established analysis practices and proposes a more principled approach to extract signal in SANS datasets. Better analysis methods are needed by experimentalists vying to measure signals ever more obscured by noise. As such, this papers answer Rutherford's call for better experiments to alleviate the need of statistics[1] by offering better statistics to analyze an existing experiment.

There are three aspects of SANS data analysis worth further comments: the need to model the signal in the space of the observations, ongoing calibration of the instrument, and a look at designing future SANS experiments.

Modeling. Raw SANS experimental data consist of pixel counts $N_{x,y}$ in the xy-plane, whose intensity is related to the scattering vector $\vec{Q}$ (see Figure 5 in Hogg et al. (2010)). Standard analysis (see Kline (2006) for example), transforms the xy-plane into $\vec{Q}$ before fitting the model by minimum χ^2. A better approach, advocated in this paper, is to transform the model defined as a function of $\vec{Q}$ into an expectation counts $\lambda_{x,y}$ in each pixel in the xy-plane.

There are several advantages to bringing the model into the space of observable data. First, it enables either a Bayesian or maximum likelihood type analysis that take advantage of the Poisson assumption for the raw pixel counts. Second, it makes possible to graphically explore the goodness-of-fit of the estimated model by displaying the residuals

$$R_{x,y} = \sqrt{N_{x,y}} - \sqrt{\hat{\lambda}_{x,y}}.$$

Finally, bootstrap samples for the data at hand are easily generated by drawing, for each pixel, the random variables

$$M_{xy}|N_{xy} \sim \text{Binomial}(N_{xy}, p),$$

for some $p \in (0, 1)$. Since marginally M_{xy} is Poisson distributed with attenuated intensity $p\lambda_{xy}$, one can analyze that data in the same way as the original counts. And since $N_{xy} - M_{xy}$ is Poisson distributed with mean $(1-p)\lambda_{xy}$, independent of M_{xy}, this opens the door to Bayesian model checking using the inferred predictive distribution for $N_{xy} - M_{xy}$.

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[1]"If you need statistics, you ought have done a better experiment", Barron Rutherford

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Calibration. The calibration of measurement instruments is an integral part of many modern experiments in the physical sciences. It involves characterizing the systematic effects arising from the measurement process, slowly varying effects, called drifts, that occur over the course of the experiment, and sample to sample random effects. The traditional approach to calibrate SANS experiments first estimates the baseline, and then uses that estimate to correct subsequently the data from the sample. The presented framework has many nice features, one of which I will elaborate on.

It is important to realize that calibration of an instrument is an ongoing process, and hence estimation of the baseline should not be undertaken *de novo* each time an experiment is performed. The Bayesian framework makes it possible to accumulate knowledge about the baseline of an instrument from periodic calibration experiments by viewing the posterior for the calibration parameters as the prior of these parameter for the next experiment.

Such an approach requires one to divide the systematic effects into fixed effects (for example the flux absorber, if it is fixed to the detector) and into random effects (for example the sample holder, if its position is changed from one experiment to the next). While the resulting analysis becomes more complex, it enables the accumulation over time of information about the baseline that results in more informative priors.

Design. Magnetization of a sample can be explored using polarized SANS experiments (Fitzsimmons et al. 2007). These experiments aim at measuring subtle differences in the scattering of *spin up* and *spin down* polarized neutrons. The framework presented in this paper is easily adapted to these experiments. However, since we seek to compare the response of the same sample to different beams, we have the opportunity to design experimental protocols that yield better paired comparisons. One such technique is to alternate during the course of the experiment the polarization of the beam. The second technique, still experimental (Fitzsimmons 2010) is to split the beam. These two techniques are not the approaches to control known sources of experimental variations. But they point the way that it is possible to estimate very small signals in SANS experiments. It is my hope that continued collaborations between statisticians and experimentalists will not only improve the analysis of SANS datasets, but impact the underlying experimental protocols, and to ultimately improve our ability to do science using small angle neutron scattering experiments.

In conclusion, the authors of this paper are to be commended for introducing statisticians to a fascinating topic in experimental physics, and physicists to modern data analysis methods.

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