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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 nano-particles. 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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