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Bayesian Inference in MANTID – An Update

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Abstract. In the context of neutron science, Bayesian inference methods have been recently implemented within the MANTID framework [Monserrat D *et al.* 2015 *J. Phys. Conf. Ser.* **663** 012009 (2015)]. In this contribution, we highlight the advantages of this software package for robust data analysis and subsequent model selection. To this end, we use the celebrated Rosenbrock function to illustrate its merits and strengths relative to *classical* fitting algorithms. We also introduce the latest additions implemented in MANTID, with a view to increasing its user friendliness as well as stimulating wider use. These include simulated-annealing schemes to reduce the need for initial guesses, as well as new options for multidimensional fitting.

1. Reverend Bayes to the Rescue

Data fitting is very often a key step in the scientific method. In the context of neutron science, the analysis of Quasielastic Neutron Scattering (hereafter QENS) data is a good case in point, as the measured response almost invariably consists of the cumulative contribution of partially overlapping signals convolved with the instrument resolution in the presence of (typically) unwanted features such as backgrounds and/or so-called 'spurions.' In this situation, a robust analytical description of a given experimental data set requires the use of several and often complex spectral functions, whose precise number and associated line shapes carry vital information on the nature of the underlying properties of the material under investigation. In the language of data analysis and statistics, we are faced with a problem in *model selection*.

Using the conceptual framework originally introduced by Sivia and Skilling [1], previous work has focused on the development of a Fitting Algorithm for Bayesian Analysis of DAta (FABADA) [2, 3]. This algorithm uses an adaptive Markov Chain Monte Carlo (MCMC) method to effect Bayesian model selection, and it is applicable to any type of data. More recently, FABADA has been implemented within the MANTID framework [4], as described in more detail in Refs. [5, 6, 7]. Beyond its well-established applicability to analyse QENS experiments [8, 9, 10], FABADA in MANTID (hereafter FIM) has also found recent use in the interpretation of Compton and mass-selective neutron-scattering data, techniques which in many respects suffer from a similar degree of spectral congestion as QENS [11, 12].

In what follows, we outline the primary advantages of FIM in its current incarnation, as well as give a brief description of the most recent additions to this software package.
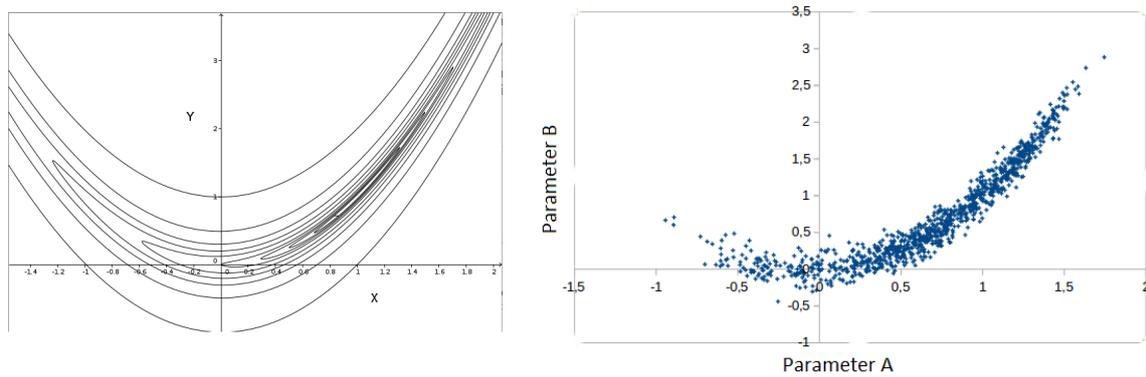
Figure 1. Contours of Rosenbrock function (**left**) and FIM converged-chain points (**right**) for that function described in the main text (for $a = 1$ and $b = 100$). A and B are fitting parameters of fitting function f(x|A,B).

2. Advantages of FABADA in MANTID – A Quick Dive

FIM aims to provide a user-friendly platform to implement Bayesian analysis with an emphasis on neutron-scattering data of any kind. In addition, the MANTID framework contains a plethora of features for the further visualisation and analysis of FIM output, including its much-needed integration with other neutron-focused algorithms and data workflows.

On a more technical front, FIM uses the natural tendency of adaptive MCMC methods to explore the entire parameter space with a (mathematically proven!) [2, 13] tendency to reach the global minimum irrespective of dimensionality. The method also yields a histogram for the *a posteriori* Bayesian parameter distributions, not just the optimal values available in widely used minimisation packages based on linear or non-linear methods, *e.g.,* Levenberg-Marquardt algorithms. This feature is a crucial one, as it enables rigorous model selection via an assumption-free analysis of the underlying Probability Density Functions (PDFs). Such an analysis can deal quite naturally with any general χ^2 landscape, including multimodal and asymmetric PDFs. These PDFs typically challenge the realm of applicability of *classical* fitting algorithms, particularly when dealing with sparse data as those arising from low-count-rate techniques. FIM can deal with these cases by simply replacing the associated cost function by suitable alternatives, and work is underway to automate these possibilities.

Figure 1 illustrates the current capabilities of FIM using the Rosenbrock function $R_{a,b}(x, y) = (x - a)^2 + b(x^2 - y)^2$. This seemingly simple function is widely used to test the robustness and reliability of minimisation algorithms to reach global minima. Standard minimisers including non-linear ones like Levenberg-Marquardt can struggle with this case owing to the non-convex nature of the χ^2 landscape, whereas FIM easily samples parameter space as well as can identify the valley minimum via the use of simulated annealing techniques, as explained in more detail below.

3. Latest Additions

3.1. Simulated Annealing

All fitting algorithms require an initial guess of all parameters, and this condition can cause serious convergence issues. FIM depends far less strongly on this choice, as MCMC methods have the tendency to explore the entire parameter space with little bias – *i.e.,* parameter sets characterised by a higher cost function (typically the χ^2) have a non-zero probability, thus enabling escape from local minima. In this situation, any χ^2 barrier towards the global minimum may be overcome provided enough time is spent exploring parameter space.
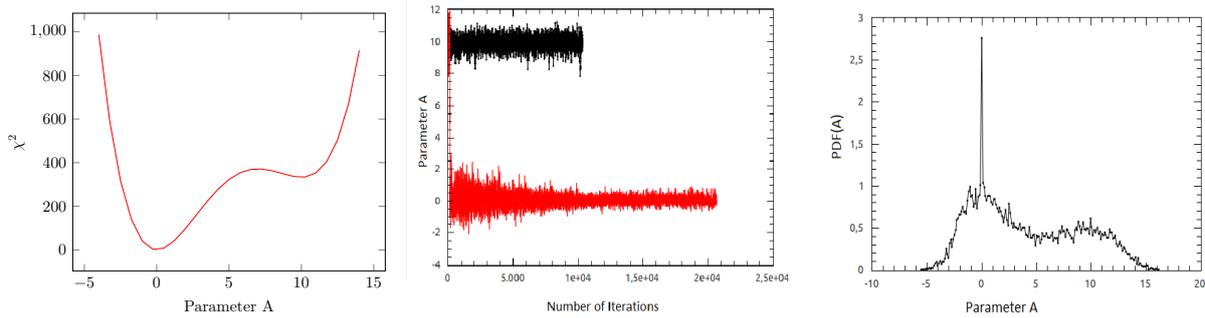
Figure 2. Simulated annealing in FIM: (**left**) χ^2 landscape; (**center**) convergence of *classical* fitting algorithms (black, local minimum) and FIM (red, absolute minimum) using an annealing temperature of 10; and (**right**) resulting PDF from FIM, showing its clear multimodal character.

To accelerate this process, FIM has been modified to include a simulated annealing option that allows for efficient jumps across χ^2 barriers of arbitrary height. In essence, this procedure works by multiplying the cost function by a constant that serves to flatten χ^2 features, therefore enabling an easier exploration of the landscape. This procedure is particularly useful when an initial guess is unavailable. In addition, it can quantify how robust parameter estimates for the location of the minimum are using the associated PDFs. These notions find a familiar analogy in thermal physics, where such a constant may be considered the temperature of the system dictating the total number of accessible states. In this vein, the *fusion* temperature of a given minimum in χ^2 space can be used to define a quantitative criterion for the robustness of a fit – in many respects, this is quite a profound connection between energy landscapes (the realm of physics) and χ^2 distributions (the realm of statistics). Figure 2 provides a simple illustration of simulated annealing in FIM. The model has been constructed to have the χ^2 landscape shown on the left, characterised by the presence of both a global and a metastable basin. The center panel shows how a sophisticated *classical* fitting algorithm such as Levenberg-Marquard gets stuck in the latter, whereas FIM can reach the global minimum without much difficulty. The figure on the right shows the associated PDF obtained with FIM, illustrating its intrinsic multimodal character.

3.2. Multidimensional Fitting
The ability to perform multidimensional fits with FIM has also been developed and preliminary tests have been performed. Using this option, it is possible to fit data collected as a function of several variables in a simultaneous fashion, *e.g.,* spatial dimensions or momentum- and energy-transfers, or parametrically as a function of external stimuli such as temperature or pressure. As example, Fig. 3 shows the uncertainties from a FIM fit to a two-dimensional Gaussian. Amongst a number of applications, we anticipate that this fresh addition to FIM will enable the use of the entire dynamic structure factor to implement model selection, as recently demonstrated in Ref. [8].

4. Outlook
Following its introduction in 2015, FIM continues to grow and evolve. Simulated annealing and multidimensional fitting constitute the latest additions to this software package and extensive testing of these capabilities is currently underway. Looking further into the future, extensions to FIM include: dealing with sparse, low-count-rate data in a statistically rigorous fashion; the definition of quantitative criteria for a systematic analysis of the information content (and associated correlation) of the underlying PDFs; the development of a library of models starting with those typically used for the analysis of QENS and Compton data; or the use of genetic
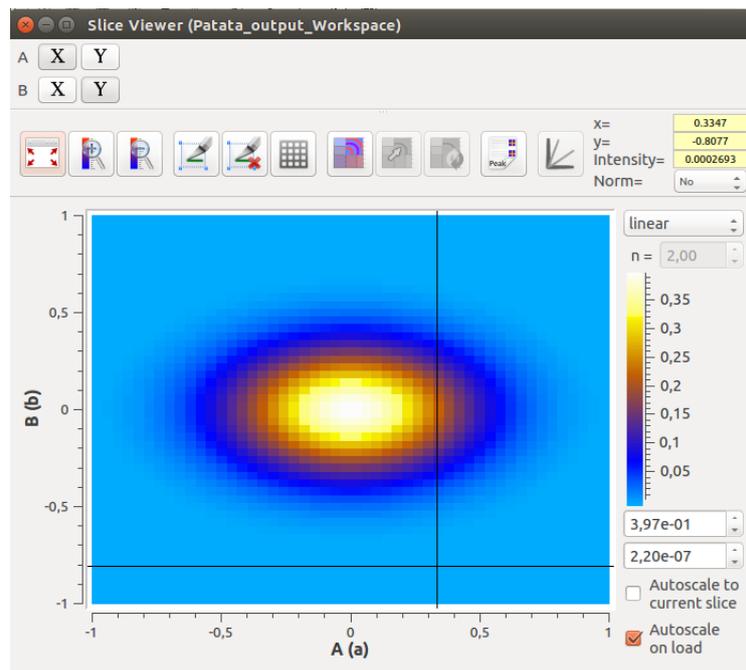
Figure 3. A snap shot of the uncertainties of two fitting parameters, A and B, obtained after multidimensional fitting with FIM to a two dimensional function. The value of χ^2 is presented by colour map. See text for more details.

algorithms to increase overall efficiency. All in all, the primary objective behind these efforts is to develop a multi-purpose state-of-the-art tool for the intuitive and robust analysis of complex neutron data.

References
[1] Sivia D and Skilling D 2006 *Data Analysis: A Bayesian Tutorial* (Oxford University Press).
[2] Pardo LC, Rovira-Esteva M, Busch S, Moulin JF and Tamarit JLl 2011 *Phys. Rev. E* **84** 046711.
[3] Pardo LC, Rovira-Esteva M, Busch S, Ruíz-Martín MD and Tamarit JLl 2011 *J. Phys. Conf. Ser.* **325** 012006.
[4] The latest version of the MANTID software is available from `dx.doi.org/10.5286/SOFTWARE/MANTID`
[5] For an up-to-date tutorial of FIM to analyse QENS data, see `www.mantidproject.org/Fitting_QENS_using_Bayesian_Routine_FABADA`
[6] Monserrat D, Vispa A, Pardo LC, Tolchenov R, Mukhopadhyay S and Fernandez-Alonso F 2015 *J. Phys. Conf. Ser.* **663** 012009.
[7] D. Monserrat, *BSc Thesis* (Universitat Politècnica de Catalunya, Spain, 2016). WEB: `epubs.stfc.ac.uk/work/24224303`
[8] Vispa A, Busch S, Tamarit JLl, Unruh T, Fernandez-Alonso F and Pardo LC 2016 *Phys. Chem. Chem. Phys.* **18** 3975.
[9] Fernandez-Alonso F, McLain SE, Taylor JW, Bermejo FJ, Bustinduy I, Ruiz-Martin MD and Turner JFC 2007 *J. Chem. Phys.* **126** 234509.
[10] Fernandez-Alonso F, Bermejo FJ, McLain SE, Turner JFC, Molaison JJ and Herwig KW 2007 *Phys. Rev. Lett.* **98** 077801.
[11] Krzystyniak M, Drużbicki D, Romanelli G, Gutmann MJ, S Rudić, Imberti S and Fernandez-Alonso F 2017 *Phys. Chem. Chem. Phys.* `dx.doi.org/10.1039/C7CP00997F`
[12] Romanelli G and Krzystyniak M 2016 *Nucl. Instr. Meth. Phys. Res. A* **819** 84.
[13] Soren Fiig Jarner, Ernst Hansen, 2000 *Stoch. Proc. Applic.* **85** 341.