Numerical Integration Precision Studies for Maximum Likelihood Fits

Maximum likelihood fits are ubiquitous in experimental high energy physics (HEP). They often calculate event-by-event un-normalized probability density functions (PDFs) and then calculate normalization integrals numerically. For multi-dimensional normalization integrals, the distribution of points within the relevant phase space where the PDF is evaluated often differs from that of the data set. In such cases, a lack of precision in calculating the normalization integrals can introduce a bias in the final results, a mis-estimation of the statistical errors reported by a fit, or both. Equally problematic, it can lead to fit instability and lack of convergence. As the precision of numerical integrals increases as $\sqrt{n}$, calculating these with sufficiently high precision can become much more computationally expensive than calculating the un-normalized likelihood values for the data themselves.

- The first goal of this project will be to produce a software toolkit to study the precisions of numerical integrals used in several multi-dimensional HEP fits and determine how the level of precision affects the biases and precisions of the parameters extracted by the fit. This work will build on the parallel function evaluation packages GooFit and Hydra.
- The second goal of this project will be to instrument the MINUIT fitting engine used most commonly in HEP to allow it to report the precisions of numerical integrals it uses, and indicate how this might affect fit results.
- The third goal of the project will be to implement better methods for evaluating normalization integrals in GooFit, specifically to replace some of the most computationally expensive parts of amplitude analyses of multi-body decays of heavy mesons. These implementations will be based on those found in Hydra.

The physics focus of this work will be amplitude analyses of heavy meson decays. These decays allow sensitive searches for new physics. The study of such processes requires multi-dimensional amplitude fits. Normalization integrals are typically done numerically, using Monte Carlo methods. Achieving good precision can be computationally expensive, especially when the PDFs involve rapidly-varying functions. An example is a decay amplitude with a very narrow resonance such as the $\phi(1020)$.

The problem of precision and stability of the PDFs numerical integration, often overlooked by analysts, must be addressed in the treatment of large data sets such as those collected by the LHC experiments. Very high precision integration using existing toolkits can be unaffordably expensive in terms of CPU time. In many practical applications, the numerical integration of the PDFs must be performed at every step during the minimization of the logarithm of the likelihood. This is particularly costly when the number of fit parameters is large ($\mathcal{O}(10^2)$), for instance, when the analysis makes use of the so called Model-Independent Partial Wave Analysis (MIPWA) technique. In this approach, part of the PDF is parameterized as a generic complex function to be determined directly from the data. The energy spectrum is divided into tens of bins and, at each bin edge, the function is defined by two real parameters. An interpolation defines the value of the PDF at any point of the spectrum. The optimum set of parameters at each bin edge is determined by the fit. Other types of analysis exploit the angular distribution of the decay products, often using the helicity formalism, to study effects of the violation of the combined Charge conjugation-Parity (CP) symmetry.

The principal mentor for this project will be Dr. Henry Schreiner from the University of Cincinnati. In addition, the student will collaborate with Prof. Michael Sokoloff from the University of Cincinnati, Prof. Alberto Reis from the Brazilian Centro Brasileiro de Pesquisas Físicas, and Prof. Liang Sun from Wuhan University. The work will be done while in residence in CERN, Switzerland.

Deliverables and Milestones

This project will extend over 12 weeks. The student will work with the mentors to develop a toolkit to test different integration methods in multi-dimensional HEP fits to test the affect of precision on the final extracted parameters. These tools will be made available for users of Minuit and GooFit or Hydra. For the following plan, it will be assumed that the code will target GooFit analyses with Hydra potentially being used for numerical integration, but the target could change to Hydra analyses instead.

The final (but absolutely critical) deliverable will be the documentation.

Weeks 1-2 Review the work done by Liang Sun and reproduce some of his results:

- Generate samples of 100K events using the isobar model presented at Charm 2016 [ref. 10 of Liang's CHEP paper].
- Study the precision of normalization integrals calculated using brute force MC integration for increasingly large samples of events in the normalization integral. For each sample size, generate 100 integrations; plot the value of the integral; determine the rms width. (Doing this will require choosing a maximum value for the PDF; it makes complete sense to use the value at the peak of the ϕ multiplied by 1.10.)
- For comparison, do essentially the same thing, but artificially increasing the width of the ϕ by a factor of 5.

Weeks 3-4 Fit MC samples using isobar and MIPWA models

- Perform isobar fits of Monte Carlo samples generated with the isobar model.
- Repeat the MIPWA studies reported by Liang Sun in his CHEP 2016 paper, arXiv 1703.03284v2.

Weeks 5-6 Replace brute force Monte Carlo integration with different integration schemes.

- Use Meerkat to generate Monte Carlo samples based on the observed data to use in numerical integration.
- use Vegas-type importance sampling following Hydra. (This uses steepness of gradients as well as absolute rates to define importance for sampling.)
- use Gaussian smoothing as implemented in Hydra to improve the precision of the integrals. This can be done for both types of importance sampling tested above.

Weeks 7-8 Prepare and test elements of a community toolkit.

- Build a tool targeting the MINUIT2 fitter to allow others to perform tests similar to above, with quantifiable comparisons to the expected fitting precision.
- Test using $B \to K^- K^+ K^+$ model that mimics data.

Weeks 9-10 Add the most effective integration techniques to GooFit.

Weeks 11-12 Prepare comprehensive documentation produced during the project. This would be available in some publicly accessible place, such as a GitBook hosted on `GitLab.com`.