Monte-Carlo fitting: the spectrum expansion.

$\mathcal{TWIST}$ Technical Note #80

Andrei Gaponenko

April 28, 2003

Abstract

This note derives a parametrization of a reconstructed spectrum in terms of deviations of parameters of the corresponding "true" spectrum. It also explains how to obtain all the terms involved using Monte-Carlo integration.

Introduction

The problem at hand: there is a parametrized theoretical PDF $f(x';\varpi)$, $x' \in \Omega_0$, ϖ are the parameters. In $\mathcal{TWIST}$ x may be, for example, $\{\text{energy}, \cos(\theta)\}$, or just $\{\text{energy}\}$, depending on the study. Correspondingly, $\varpi \equiv \{\rho, \eta, P_\mu\xi, \delta\}$, or $\varpi \equiv \{\rho, \eta\}$.

In an experiment instead of f we get some "observed" distribution $f_{\text{obs}}(x;\varpi)$ which is affected by the detector and reconstruction. Using theoretical f we can calculate $f_{\text{predicted}}(x;\varpi)$ for a fixed ϖ to compare it with f_{obs}. However the calculation is expensive (requires a high statistics Monte-Carlo). We want an easier way to get $f_{\text{predicted}}(x;\varpi)$ for *any* ϖ, at least in a small range of parameters, to try to match the predicted spectrum to the observed one by changing ϖ.

An "obvious" solution, calculating $f_{\text{predicted}}(x;\varpi)$ for two close values of ϖ and interpolating, in practice does not work, since it involves measuring a small difference of two large numbers, where the statistical error gets multiplied by $1/|\Delta\varpi|$. Going this way would require statistics of $N \times |\Delta\varpi|^{-2}$ events instead of N, and $\Delta\varpi$ is small. It turns out we can do a better job using our knowledge of derivatives of the theoretical distribution.

All spectra dealt with in this note are statistical expectations. Doing an actual fit, besides knowing the mean, requires also calculating a likelihood, or a χ^2, and is not discussed here.

Spectrum shape

If there is an event at x', the probability to get it reconstructed in volume dx around x is $K(x,x')\,dx$. This is the definition of response function K. This definition combines effects of the detector and reconstruction. Integrating over x in bin i of the spectrum histogram, we get a "binned" response function $K_i(x')$, that is, the probability to get the reconstructed event in bin i.

For a dataset with N' true decays, the expected number of events reconstructed in bin i is:

$$N_i(\varpi) = B_i + N' \int\limits_{\Omega_0} K_i(x')\, f(x';\varpi)\, dx' \tag{1}$$

where B_i is the background, $f(x';\varpi)$ is the true distribution of decays, and Ω_0 is the whole kinematically allowed phase space. Often we have an analytical expression for the theoretical distribution representing f only up to a normalization factor:

$$f(x';\varpi) = A(\varpi)\, F(x';\varpi), \qquad \int\limits_{\Omega_0} f(x';\varpi)\, dx' \equiv 1, \tag{2}$$

we know the F but do not know the A. (Of course A can be calculated numerically.)

$\mathcal{TWIST}$ measures the shape of the spectrum. We can get rid of the absolute count by normalizing N_i to the total number of reconstructed events in fiducial volume Ω:

$$n_i(\varpi) = N_i(\varpi)/N(\varpi), \qquad \text{where} \quad N(\varpi) = \sum_{\Omega} N_i(\varpi). \tag{3}$$

A change in parameters ϖ modifies spectrum shape n_i as

$$n_i(\varpi + \Delta\varpi) - n_i(\varpi) = \Delta\varpi\, \frac{1}{N}\frac{\partial N_i}{\partial \varpi} - n_i(\varpi)\, \Delta\varpi \sum_{\Omega} \frac{1}{N}\frac{\partial N_i}{\partial \varpi} + \mathcal{O}(\Delta\varpi^2) \tag{4}$$

Using (1)–(3) we can express the derivative on the right hand side as:

$$\begin{aligned}\Delta\varpi \frac{1}{N}\frac{\partial N_i}{\partial \varpi} &= \frac{N'}{N} A(\varpi)\, \Delta\varpi \int\limits_{\Omega_0} K_i(x')\, \frac{\partial F(x';\varpi)}{\partial \varpi}\, dx' \\ &\quad + \frac{N_i}{N}\, \Delta\varpi\, \frac{1}{A(\varpi)}\frac{\partial A}{\partial \varpi} - \frac{B_i}{N}\, \Delta\varpi\, \frac{1}{A(\varpi)}\frac{\partial A}{\partial \varpi} + \mathcal{O}(\Delta\varpi^2).\end{aligned} \tag{5}$$

Also,

$$\Delta\varpi\, \frac{1}{A(\varpi)}\frac{\partial A}{\partial \varpi} = -A(\varpi)\, \Delta\varpi \int\limits_{\Omega_0} \frac{\partial F(x';\varpi)}{\partial \varpi}\, dx'. \tag{6}$$

and

$$A^{-1}(\varpi) = \int\limits_{\Omega_0} F(x';\varpi)\, dx', \tag{7}$$

Analytical expressions for F and $\partial F/\partial\varpi$ are known, so there are many possible ways to calculate integrals (6)–(7). The integral (5) contains an unknown response function K, and has to be evaluated from Monte-Carlo. It is convenient to calculate (6)–(7) by Monte-Carlo integration as well.

Doing the integrals

A definite integral of a bounded non-negative function $g(x')$ can be evaluated using the acceptance-rejection method: choose a $Y_{\max} \geq \sup_{x'\in\Omega_0} g(x')$ and sample N_{thrown} points $\{x', y\}$ from a uniform distribution on $\Omega_0 \times [0, Y_{\max}]$. Call a point accepted if $y < g(x')$. Then

$$\int\limits_{\Omega_0} g(x')\, dx' \approx \frac{N_{\text{acc}}}{N_{\text{thrown}}}\, Y_{\max} \int\limits_{\Omega_0} dx'. \tag{8}$$

where N_{acc} is the count of accepted points. That recipe is applicable for evaluating (7). For a more general $g(x')$

$$\int\limits_{\Omega_0} g(x')\, dx' = \int\limits_{\Omega_0} g^+(x')\, dx' - \int\limits_{\Omega_0} g^-(x')\, dx' \tag{9}$$

where g^+ and g^- are non-negative functions:

$$g^+(x') = \begin{cases} g(x') & \text{if } g(x') \geq 0, \\ 0 & \text{otherwise,} \end{cases} \qquad g^-(x') = \begin{cases} |g(x')| & \text{if } g(x') < 0, \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

Then from (8)

$$\int\limits_{\Omega_0} g(x')\, dx' \approx \frac{N^+_{\text{acc}} - N^-_{\text{acc}}}{N_{\text{thrown}}}\, Y_{\max} \int\limits_{\Omega_0} dx', \tag{11}$$

where

$$Y_{\max} \geq \sup_{x'\in\Omega_0} |g(x')|, \tag{12}$$

$$y < g^+(x') \quad \text{for} \quad N^+_{\text{acc}}, \tag{13}$$

$$y < g^-(x') \quad \text{for} \quad N^-_{\text{acc}}. \tag{14}$$

The integral in (6) can be calculated this way.

To evaluate the integral in (5) we can use the following procedure: take "generating function" $g(x') = \partial F(x'; \varpi)/\partial\varpi$ and sample $\{x', y\}$ from a uniform distribution as before. For every point accepted according to (13) or (14) use x' to define kinematic of an event in GEANT, simulate and reconstruct the event. If the event passed the whole analysis chain and landed in bin i, count it as $N_i^+[\frac{\partial F}{\partial\varpi}]$ or $N_i^-[\frac{\partial F}{\partial\varpi}]$. Then

$$\int\limits_{\Omega_0} K_i(x')\, \frac{\partial F(x';\varpi)}{\partial\varpi}\, dx' = \frac{N_i^+[\frac{\partial F}{\partial\varpi}] - N_i^-[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]}\, Y_{\max}[\tfrac{\partial F}{\partial\varpi}] \int\limits_{\Omega_0} dx' \tag{15}$$

and

$$\Delta\varpi\,\frac{1}{N}\frac{\partial N_i}{\partial\varpi} = \Delta\varpi\,\frac{Y_{\max}[\frac{\partial F}{\partial\varpi}]}{Y_{\max}[F]}\,\frac{N_{\text{thrown}}[F]}{N[F]} \times \left\{ \frac{N_i^+[\frac{\partial F}{\partial\varpi}] - N_i^-[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]} - \frac{N_i[F]-B_i}{N'[F]}\,\frac{N'^+[\frac{\partial F}{\partial\varpi}] - N'^-[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]} \right\} + \mathcal{O}(\Delta\varpi^2). \quad (16)$$

N' here, as before, denotes the number of "true" decays, that is, accepted in generation but not necessarily passed through the analysis. The argument in the square brackets indicate what generating function was involved. For example, $N_i[F] \equiv N_i$, and $N'[F] \equiv N'$ from (1). The numbers N, N_i, $N_i^{\pm}$, N' , $N'^{\pm}$ are to be understood as statistical expectations.

Substituting (16) into (4) and introducing

$$N_i[\tfrac{\partial F}{\partial\varpi}] = N_i^+[\tfrac{\partial F}{\partial\varpi}] - N_i^-[\tfrac{\partial F}{\partial\varpi}], \qquad N'[\tfrac{\partial F}{\partial\varpi}] = N'^+[\tfrac{\partial F}{\partial\varpi}] - N'^-[\tfrac{\partial F}{\partial\varpi}], \quad (17)$$

we finally get

$$n_i(\varpi+\Delta\varpi) - n_i(\varpi) = \Delta\varpi\,\frac{Y_{\max}[\frac{\partial F}{\partial\varpi}]}{Y_{\max}[F]}\,\frac{N_{\text{thrown}}[F]}{N[F]} \times \left\{ \frac{N_i[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]} + \frac{B_i}{N'[F]}\,\frac{N'[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]} - \frac{N_i[F]}{N[F]}\,\frac{N[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]} - \frac{N_i[F]}{N[F]}\,\frac{B}{N'[F]}\,\frac{N'[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]} \right\} + \mathcal{O}(\Delta\varpi^2). \quad (18)$$

where $B = \sum_{i\in\Omega} B_i$.

We can choose $Y_{\max}[\frac{\partial F}{\partial\varpi}] = Y_{\max}[F]$ and process the "base" spectrum F and derivative spectra $\frac{\partial F}{\partial\varpi}$ in a single pass $N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}] \equiv N_{\text{thrown}}[F]$. Then from (18) one can see that the reconstructed derivative spectra could be normalized to the reconstructed base spectrum from the same pass, and we would not need to know N_{thrown}. However computationally it's more efficient to produce a base spectrum and each derivative in separate runs.

Introducing the efficiency

$$\mathcal{E}(\varpi) = Y_{\max}[F]\,\frac{N[F]}{N_{\text{thrown}}[F]} \quad (19)$$

of the mapping of $\Omega_0 \times [0, Y_{\max}]$ into Ω, the integral of $\partial F/\partial\varpi$

$$\mathcal{D}(\varpi) = Y_{\max}[\tfrac{\partial F}{\partial\varpi}]\,\frac{N'[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]}, \quad (20)$$

and normalized spectra

$$\nu_i(\varpi) = Y_{\max}[\tfrac{\partial F}{\partial\varpi}]\,\frac{N_i[\frac{\partial F}{\partial\varpi}]}{N_{\text{thrown}}[\frac{\partial F}{\partial\varpi}]}, \qquad \beta_i = \frac{B_i}{N'[F]}, \quad (21)$$

we can re-write (18) as

$$n_i(\varpi + \Delta\varpi) = \left[1 - \sum_{\alpha=1}^{m} \Delta\varpi_\alpha \, \mathcal{E}^{-1}(\nu^\alpha + \beta\mathcal{D}^\alpha)\right] n_i(\varpi)$$
$$+ \sum_{\alpha=1}^{m} \Delta\varpi_\alpha \, \mathcal{E}^{-1}(\nu_i^\alpha + \beta_i\mathcal{D}^\alpha) + \mathcal{O}(\Delta\varpi^2) \quad (22)$$

Here the index $\alpha = \overline{1,m}$ numbering the components of ϖ is shown explicitly, $\beta = \sum_{i\in\Omega}\beta_i$, and $\nu^\alpha = \sum_{i\in\Omega}\nu_i^\alpha$.

So, a "shifted" spectrum $n_i(\varpi + \Delta\varpi)$ can be represented as a linear combination of a "base" spectrum $n_i(\varpi)$ and m "derivative" spectra according to (18) or (22). The derivative spectra can only be obtained for simulated data. For a real measurement of Michel parameters the "shifted" spectrum is the experimental one, and the "base" comes from a simulation. For systematic studies MC+MC or data+data combinations of shifted+base spectra are useful, where "shifted" and "base" spectra are obtained under different conditions. (I.e. the assumption that K is the same is broken.)

The technique described above assumes independently reconstructed decays (the limit of zero beam intensity). If there is more than one muon decay in an event, they are not independent any more, and, strictly speaking, our MC integration formulas become invalid. Another interpretation is that reconstruction of one decay from an event is affected by the presence of the second one, so response function K starts depending on ϖ. This effect can be investigated using a data-to-data or MC-to-MC comparison as any other systematic.

If muon decay spectrum is parametrized in terms of $\{\rho, \eta, P_\mu\xi, P_\mu\xi\delta\}$, the quadratic terms $\mathcal{O}(\Delta\varpi^2)$ are absent, and ν_i^α and $\mathcal{D}$ do not depend on ϖ. If we use the $\{\rho, \eta, P_\mu\xi, \delta\}$ parametrization, the base spectrum is required to be close to the shifted one. The constraint is not too tight: it's enough to set $P_\mu\xi$ and δ for the base spectrum right within 1% to make the only quadratic term $\Delta P_\mu\xi\,\Delta\delta \approx 10^{-4}$.