Estimation of Goodness-of-Fit in Multidimensional Analysis Using Distance to Nearest Neighbor *

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(Dated: October 31, 2018)

Abstract

A new method for calculation of goodness of multidimensional fits in particle physics experiments is proposed. This method finds the smallest and largest clusters of nearest neighbors for observed data points. The cluster size is used to estimate the goodness-of-fit and the cluster location provides clues about possible problems with data modeling. The performance of the new method is compared to that of the likelihood method and Kolmogorov-Smirnov test using toy Monte Carlo studies. The new method is applied to estimate the goodness-of-fit in a $B \to Kl\ell$ analysis at BaBar.

PACS numbers: 02.50.-r, 02.50.Ng, 02.50.Sk.

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* Work partially supported by Department of Energy under Grant DE-FG03-92-ER40701.
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1. INTRODUCTION

Fits are broadly used in analysis of particle physics experiments. If sufficient statistics is accumulated, one usually plots observed data as a histogram and overlays an expected histogram or modeling function. The goodness-of-fit is then estimated by taking the deviation of the observed number of events in each bin from the expected number of events in the same bin, summing the squares of these deviations to form a $\chi^2$ value and hence compute a significance level. This procedure assumes that the bin contents are normally distributed, which is true only asymptotically in the large statistics limit. In low-statistics experiments, one typically observes zero or just a few events per bin, and this procedure does not produce a reliable result. One must then use other methods. Unbinned maximum likelihood methods, discussed below, have been recently used in such situations in Babar and elsewhere. We also discuss Kolmogorov-Smirnov test, another well-known method.

In this note, we concentrate on the most general problem: how to test a distribution in question against every reasonable alternative hypothesis. In other words, the null and alternative hypotheses are stated as follows:

$H_0$ : the observed data obey the expected distribution.

$H_1$ : the observed data obey some other unknown but plausible distribution.

The goodness-of-fit, $1 - \alpha$, is defined as the confidence level of the null hypothesis, and $\alpha$ is therefore a Type I error. We remind the reader that the Type II error is traditionally defined as the probability of accepting the null hypothesis if the alternative hypothesis is true.

This definition of the problem conforms with the standard $\chi^2$ test of binned data. Indeed, the $\chi^2$ test computes discrepancy between expected and observed probability density functions (pdf’s) without imposing constraints on the alternative hypothesis. We do not discuss examples, where the alternative hypothesis $H_1$ can be stated in a more specific form, e.g., testing normality versus uniformity. Our goal is to propose a new generic procedure applicable to unbinned fits.

It is not possible to design a versatile procedure applicable to all problems. For example, we can always choose the alternative distribution to be a set of $\delta$-functions positioned precisely at the observed experimental points. In this case, the null hypothesis is inferior to the alternative hypothesis and the null hypothesis is rejected. This simply reflects the fact that the Type II error is undefined for the generic test stated in the previous paragraph. We would like to keep our procedure as generic as possible. Yet if more information about the alternative hypothesis is available, it should be possible to design a more powerful test for this specific alternative.

We note that the standard $\chi^2$ binned test computes an average deviation of observed data from the expected density. However, in many experiments it is useful to focus on the maximal deviation instead of the average one. Consider, for example, fitting a one-dimensional histogram divided into 20 bins in the range $[-10, 10]$ to the sum of a standard normal pdf $N(0, 1)$ with zero mean and unit variance and a uniform pdf, as shown in Fig. 1. The normal pdf represents signal (for example, mass of a certain resonance) and the uniform pdf represents background, with the magnitude of each component fixed to 100 entries. The $\chi^2$ deviation, computed as $\sum_{bins}(N_{\text{expected}} - N_{\text{observed}})^2/N_{\text{expected}}$, is 19.34 per 20 degrees of freedom for each of the three fits, which results in a goodness-of-fit value of 50%. Hence, the procedure treats all fits as those of equal quality. In reality, of course, the experimenter will treat each fit in a different way. The top fit will be likely considered as “good”. The middle
fit will likely raise concern about a large background fluctuation in one bin. The bottom fit will likely make the experimenter suspect that the signal is not well modeled by the normal standard pdf with an area of 100. In fact, the experimenter is not really concerned about the $\chi^2$ deviation averaged over all bins. The more interesting question is: what are the bins that give largest $\chi^2$ deviations from expected values and how probable are these deviations? The method proposed in this note is designed to answer both these questions for unbinned fits.

FIG. 1: Three fits with 50% goodness-of-fit values computed using the standard $\chi^2$ method for binned data. Top plot — the $\chi^2$ deviations are distributed uniformly over the bins; middle plot — the $\chi^2$ deviation is entirely due to one bin at the left edge of the histogram; bottom plot — the $\chi^2$ deviation is produced by the two central bins.

2. MAXIMUM LIKELIHOOD VALUE TEST

The Maximum Likelihood Value (MLV) test is laid out in the BaBar Statistics Report [1]. For any quantity $x$ that characterizes fit quality, the goodness-of-fit is given by

$$1 - \alpha = 1 - \int_{f(x|H_0) > f(x_{obs}|H_0)} f(x|H_0) \, dx ,$$

(1)
where \( x_{\text{obs}} \) is the value of \( x \) observed in the fit to the data, and \( f(x|H_0) \) is the pdf of quantity \( x \) under the null hypothesis. For the MLV test, the quantity of interest is the likelihood and so \( \mathcal{L} \) replaces \( x \) in the equation above.

By construction, the MLV test can be only used to discriminate against a specific class of alternative hypotheses. Data are fitted to the density \( f(x|\theta) \) and an estimate of the parameter \( \theta = \theta_0 \) is obtained from the fit. Then the null hypothesis \( H_0 : \theta = \theta_0 \) is tested against the alternative hypothesis \( H_1 : \theta \neq \theta_0 \). Note that the overall validity of the density \( f(x|\theta) \) is never questioned. If the data are drawn from a drastically different pdf, this test can produce a meaningless result.

Consider, for instance, fitting a one-dimensional random sample to a standard normal pdf \( N(0,1) \). In reality, however, the data are drawn from a sum of two narrow normal pdfs placed two units apart: \( N(-1,0.01) \) and \( N(+1,0.01) \), as shown in Fig. 2. Distributions of likelihood values computed under the null hypothesis for events drawn from the standard normal pdf \( N(0,1) \) and events drawn from the sum of two normal pdfs are shown in Fig. 2. Likelihood values computed under the null hypothesis \( N(0,1) \) for the sum of two narrow normal pdfs are always consistent with the null hypothesis. The procedure does not have any discriminative power and the obtained fit always produces a reasonable goodness-of-fit value, even though the null hypothesis is clearly wrong. In this example an experimenter can easily find the problem by visual comparison of the distributions, but in the real world of multidimensional distributions such a comparison would be harder to make.

Why did the MLV test fail to reject the null hypothesis for the random sample described in the previous paragraph? Because the alternative hypothesis \( H_1 \) was not “every other plausible distribution” but “another normal distribution”. The price for this assumption was a futile test. It is true that the procedure would also discriminate against certain non-normal distributions. But it would work by accident, not by design.
Another good example is a test of uniformity. Maximum likelihood methods are useless here because under uniformity the likelihood value is constant, no matter how points are distributed.¹

3. GENERIC TESTS

3.1. Outline

In the previous section, we established that the likelihood method does not address the problem stated in the Introduction. A more versatile approach is to test the null hypothesis without making specific assumptions about its alternative. We refer to such tests as “generic”.

In Section 3.2 we briefly discuss information about generic tests that can be found in the statistics literature. Then we proceed with discussion of the Kolmogorov-Smirnov test, a well-known generic approach, in Section 3.4 and propose a new method in Section 3.6. We emphasize that any generic test can be standardized by transforming the density of interest to uniform and performing a test of uniformity. The transformation to a uniform density is described in Section 3.3 and the definition of uniformity is discussed in Section 3.5. The transformation to a uniform density is not required for the Kolmogorov-Smirnov test but is essential for the proposed method. Subtleties related to the non-uniqueness of the uniformity transformation are discussed in Section 3.7.

3.2. Statistics Literature

There is a great amount of statistics literature on goodness-of-fit tests. Unfortunately, a great fraction of this literature is useless to us because of one of the following reasons:

- The discussed problem is too specific, e.g., testing one specific type of pdf against another specific type of pdf.
- Asymptotic approximations, e.g., the central limit theorem, are used.
- Authors concentrate on designing an analytic tool (inevitably based on some approximation) and dismiss MC simulation.

We, on the other hand, would like to have a generic approach for unbinned fits with small numbers of events. We can rely on MC generators; hence, analyticity of the solution is not an issue.

A well-known method that complies with these requirements is the Kolmogorov-Smirnov test. However, the Kolmogorov-Smirnov test lacks sensitivity for a broad class of alternative hypotheses.

To our knowledge, the distance-to-nearest-neighbor method proposed in Section 3.6 has not been described anywhere in the literature. As the idea seems obvious, it is quite possible that we are simply reinventing the wheel. But we hope that this wheel is worth reinventing.

¹ Unless there is an experimental point observed outside the range of definition of the uniform pdf.
3.3. Transformation to Uniform Density

Before we proceed with discussion of various methods, we note that the problem can be standardized by transforming any $n$-dimensional pdf $f$ in question to uniform. This transformation offers a number of advantages:

- All problems are described by the same formalism.
- The practical task of generating toy MC experiments is easily solved with a uniform random number generator.
- It is easy to implement this transformation numerically in the absence of an analytic model for the pdf.

Any $n$-dimensional random vector $(x^{(1)}, x^{(2)}, ..., x^{(n)})$ with a joint pdf $f(x^{(1)}, x^{(2)}, ..., x^{(n)})$ can be transformed to a vector $(u^{(1)}, u^{(2)}, ..., u^{(n)})$ uniformly distributed on an $n$-dimensional unit cube $0 \leq u^{(i)} \leq 1; \ i = 1, 2, ..., n$. This transformation is given by

$$
\begin{align*}
\begin{cases}
  u^{(1)} = \int_{-\infty}^{x^{(1)}} f_1(t, x^{(2)}, x^{(3)}, ..., x^{(n)}) dt / f_2(x^{(2)}, x^{(3)}, ..., x^{(n)}) \\
  u^{(2)} = \int_{-\infty}^{x^{(2)}} f_2(t, x^{(3)}, x^{(4)}, ..., x^{(n)}) dt / f_3(x^{(3)}, x^{(4)}, ..., x^{(n)}) \\
  \vdots \\
  u^{(n-1)} = \int_{-\infty}^{x^{(n-1)}} f_{n-1}(t, x^{(n)}) dt / f_n(x^{(n)}) \\
  u^{(n)} = \int_{-\infty}^{x^{(n)}} f_n(t) dt
\end{cases}
\end{align*}
$$

(2)

where

$$
\begin{align*}
\begin{cases}
  f_1(x^{(1)}, x^{(2)}, ..., x^{(n)}) = f(x^{(1)}, x^{(2)}, ..., x^{(n)}) \\
  f_2(x^{(2)}, x^{(3)}, ..., x^{(n)}) = \int_{-\infty}^{x^{(2)}} f_1(x^{(1)}, x^{(2)}, ..., x^{(n)}) dx^{(1)} \\
  f_3(x^{(3)}, x^{(4)}, ..., x^{(n)}) = \int_{-\infty}^{x^{(3)}} f_2(x^{(2)}, x^{(3)}, ..., x^{(n)}) dx^{(2)} \\
  \vdots \\
  f_n(x^{(n)}) = \int_{-\infty}^{x^{(n)}} f_{n-1}(x^{(n-1)}, x^{(n)}) dx^{(n-1)}
\end{cases}
\end{align*}
$$

(3)

This transformation is one-to-one for a strictly positive pdf $f(\vec{x})$.

The cumulative density function (cdf) for an $n$-dimensional uniform distribution is simply

$$
F(\vec{u}) = \prod_{i=1}^{n} u^{(i)}.
$$

(4)

3.4. Kolmogorov-Smirnov Test

A generic method broadly known to physicists is the Kolmogorov-Smirnov test. The Kolmogorov-Smirnov statistic for a random sample $\vec{x}_1, \vec{x}_2, ..., \vec{x}_N$ of $n$-dimensional vectors $\vec{x} = (x^{(1)}, x^{(2)}, ..., x^{(n)})$ with a cdf $F(\vec{x})$ is given by

$$
K_N(F) = \sup_{\vec{x} \in V_n} |F(\vec{x}) - F_{\text{obs}}(\vec{x})|,
$$

(5)

where $V_n$ is an $n$-dimensional domain for the cdf $F(\vec{x})$, and $F_{\text{obs}}(\vec{x})$ is the experimentally observed cdf. The null hypothesis is accepted if $K_N(F_0)$ is small and rejected if $K_N(F_0)$ is large, where $F_0$ is a cdf for the null hypothesis.
Because the Kolmogorov-Smirnov test compares cumulative densities, it lacks sensitivity to fluctuations within small clusters. Consider, for example, two sets of points on a unit interval $0 \leq x \leq 1$:
Set 1: $x_1 = 1/4$, $x_2 = 1/2$, $x_3 = 3/4$, $x_4 = 1$
Set 2: $x_1 = x_2 = 1/4$, $x_3 = x_4 = 3/4$
Which one of these sets looks more uniform? The Kolmogorov-Smirnov test cannot differentiate between these two because the statistic $[5]$ is $1/4$ under uniformity in both cases.

3.5. What Is “Uniform”?

In fact, the question we asked in the previous section is not so simple. Can we indeed make a statement about which set is more likely to be drawn from a uniform distribution? The answer is: it depends.

Suppose we search for a heavily-suppressed decay using BABAR data. We plot the mass distribution and we are convinced that background in our analysis is flat. We would like to know if there is an indication of any mass peaks in the plotted data. The data points in Set 1 from the previous section are equally spaced while the data points from Set 2 are grouped together in two clusters. Hence, Set 1 looks more uniform than Set 2.

Consider now another example. We have a detector that registers ionizing particles. We would like to test the randomness of the particle flux, that is, the exponentiality of the distribution of time intervals between consecutive events. However, after an event is registered, the detector becomes inactive for a certain period of time. If the expected time interval between two consecutive events is much less than the detector’s deadtime, the device will trigger at fixed time intervals. This would indicate that the process is not exponential but periodic. On these grounds, we would conclude that Set 1 looks less uniform than Set 2.

We obtained two opposite answers to the same question. Of course, the question was not the same; in effect, these were two different questions. In the first example, the vaguely stated alternative hypothesis was “presence of peaks in the data”. In the second example, it was “equidistant points on a finite interval”. We cannot design a test that gives the right answer for every possible problem. Nevertheless, it would be good to have a procedure which is more sensitive to clustering of data than the Kolmogorov-Smirnov test is.

3.6. Distance-to-Nearest-Neighbor Test of Uniformity

The idea of using the distance to nearest neighbor for a test of uniformity is not new [4, 5, 6]. For each data point, $\vec{u}_i = (u_i^{(1)}, u_i^{(2)}, ..., u_i^{(n)})$, in an $n$-dimensional unit cube we find the nearest neighbor, $\vec{u}_{ij}$, and compute the distance, $d_{ij} = |\vec{u}_i - \vec{u}_j|$. Uniformity is tested by comparing observed values of $d_{ij}$ with those expected for a uniform distribution. In a more general approach, one can use an average distance $d_i^{(m)}$ to $m > 1$ nearest neighbors. In Refs. [4, 5, 6], discussion revolves around using moments of distributions of distances $d_i^{(m)}$ as test statistics. We propose a test of uniformity based on minimal and maximal values of the distance $d_i^{(m)}$ to $m$ nearest neighbors. It is intuitively clear that such test should be more sensitive to maximal deviations of observed data from the tested pdf than the Kolmogorov-Smirnov test is.

A similar approach would be to use maximal and minimal volumes of Voronoi regions. A Voronoi region for a given observed point $\vec{u}_i$ is defined as a set of points inside the $n$-
dimensional unit cube which are closer to $\vec{u}_i$ than to any other observed point $\vec{u}_j$, $j \neq i$. Voronoi regions have been used by the Sleuth algorithm\cite{1} to search for new physics at the D0 experiment. In essence, Sleuth computes the probability of observing one data point in each Voronoi region based on the expectation value for background and marks Voronoi cells with low probabilities as candidates for a new physics signal. This method addresses the same question: how consistent are observed data with a null hypothesis, where the null hypothesis is defined as “background events only”. To a zeroth order, the volume of a Voronoi region around $m+1$ points is proportional to the average size $d_{i}^{(m)}$ of the cluster. Therefore, both methods for goodness-of-fit estimation are expected to produce similar results. This is confirmed by MC tests described in Section\ref{MC}. However, using distance to nearest neighbor is computationally simpler because the construction of Voronoi regions can be avoided.

3.7. Invariance of Test Statistic under Uniformity Transformation

The transformation to uniformity is not unique, even if we limit the problem to continuous mappings. A transformation $\vec{x} \to \vec{u}$ is continuous if two infinitely close points are mapped onto two infinitely close points, i.e., $\lim_{|\vec{x}_i - \vec{x}_j| \to 0} |\vec{u}_i - \vec{u}_j| = 0$. Consider, for example, a uniform pdf on a unit circle $f(r, \phi) = 1/\pi; 0 \leq r \leq 1, 0 \leq \phi \leq 2\pi$. The joint pdf of random variables

$$
\begin{align*}
  r' &= r \\
  \phi' &= \phi + \alpha r; \quad 0 < |\alpha| < \infty
\end{align*}
$$

(6)

is also uniform on the unit circle. However, this transformation does not conserve distance between two points. Another example is relabeling of variables $x^{(0)}$ in transformation\cite{2} for a non-factorizable pdf in $n > 1$ dimensions.

It is clear that all possible transformations to uniformity do not necessarily produce identical values either for the Kolmogorov-Smirnov statistic or the distance to nearest neighbor. Inevitably, the value of goodness-of-fit for a specific set of experimental data depends on the choice of transformation. We do not consider this circumstance as a major obstacle. In many problems, it is possible to find a reasonable transformation to uniformity that preserves the natural metric of the experiment.

In many particle physics experiments, observation variables are independent or weakly correlated. The pdf of interest is therefore factorizable or close to such. In this case, transformation\cite{2} is reduced to $u^{(i)} = F_i(x^{(0)}); i = 1, 2, ..., n$, where $F_i$ is a marginal cdf for $i$th component. The transformation above is the most obvious and natural choice. In other experiments, the pdf can be transformed to a factorizable one. For example, a two-dimensional normal pdf can be rotated to align the axes of the normal elliptic contour with the coordinate axes.

If the pdf is severely non-factorizable, one can split $n$ observation variables into $k$ mutually independent (or weakly correlated) groups with $n_i, i = 1, 2, ..., k$, variables in each group, $n = n_1 + n_2 + ... + n_k$. Within each group, variables are strongly correlated and the marginal $n_i$-dimensional pdf cannot be factorized. To obtain a test statistic invariant under relabeling of observation variables $x^{(i)}$ in transformation\cite{2}, one would have to try all $n_i!$ permutations of variables within each group. For example, the minimal distance to nearest neighbor would be chosen as the minimum of all distances to nearest neighbor in these $n_i!$ permutations. This method was proposed\cite{3} for a multidimensional Kolmogorov-Smirnov test. We simply restate it here in reference to the distance-to-nearest-neighbor approach.
4. TESTS

We consider four two-dimensional pdf's $f(x, y)$:

- normal pdf $N(\mu_X = 0, \mu_Y = 0, \sigma_X^2 = 1, \sigma_Y^2 = 1, \rho = 0)$ with zero means, unit variances and zero correlation between $x$ and $y$
- narrow normal pdf $N(0, 0, 0.25, 0.25, 0)$
- sum of two narrow normal pdf's $N(-1.3, 0, 0.01, 0.01, 0)$ and $N(+1.3, 0, 0.01, 0.01, 0)$
- uniform pdf defined on a square $-5 \leq x \leq 5; -5 \leq y \leq 5$

For each density, we run 10,000 toy MC experiments with 10 events per experiment. We use the standard normal pdf $N(0, 0, 1, 1, 0)$ as the null hypothesis (except one example, as discussed below) and plot in Fig. likelihood values $-2 \log L_0$ computed under the null hypothesis for all pdf's. Assuming the null hypothesis, we apply uniformity transformation to each MC experiment and plot values of the Kolmogorov-Smirnov statistic for all pdf's in Fig. We also plot two-dimensional distributions of maximal versus minimal distance to nearest neighbor in Fig. We use these MC distributions to estimate Type II errors for hypothesis tests at a given confidence level against each alternative to the null hypothesis. The confidence levels and errors are shown in Table 1. We repeat this exercise treating the uniform pdf as the null hypothesis and testing it against the standard normal pdf $N(0, 0, 1, 1, 0)$. This result is also shown in Table 1 and Fig.

With the definitions of the Type II error and confidence level shown in the Introduction, the smaller is the Type II error for a fixed confidence level, the more powerful is the test.

We compared results obtained by the distance-to-nearest-neighbor method to those obtained through Voronoi regions and found no significant difference.

The maximum likelihood method is very efficient for discriminating one normal pdf against another and against a uniform pdf which can be considered as a limiting case of a normal distribution with large variance. As expected, it fails to discriminate against two narrow normal pdf's because the implicit assumption of overall normality for the alternative hypothesis does not hold in this case. The distance-to-nearest-neighbor method performs better than the Kolmogorov-Smirnov approach for every test. This confirms our intuitive assumption about enhanced sensitivity of the distance-to-nearest-neighbor method to deviations of data from an expected pdf. We note that the proposed distance-to-nearest-neighbor method is versatile as it provides some level of discrimination against every alternative hypothesis, although by no means should it be expected to provide the best discrimination against every alternative hypothesis.

5. EXAMPLE: EVIDENCE FOR $B \to K^{(*)}l^+l^-$ AT BaBar

We apply the proposed distance-to-nearest-neighbor method to results of a $B \to K^{(*)}l^+l^-$ study at BaBar. In this study, eight $B \to K^{(*)}l^+l^-$ decays were investigated. Signal rate and upper limit estimates were obtained for these eight decays. We concentrate on two modes with measured signal yields: $N(B^+ \to K^+e^+e^-) = 14.4^{+5.0}_{-4.2}$ and $N(B^+ \to K^+\mu^+\mu^-) = 0.5^{+2.3}_{-1.3}$ (statistical errors only). The former can be described as a “significant measurement” while the latter can be used to set an upper limit.
FIG. 3: $-2 \log L_0$ under the null hypothesis $N(0, 0, 1, 1, 0)$ for the four pdfs discussed in the text. A histogram for the uniform pdf is not shown because it is far to the right.

TABLE I: Confidence levels (CL) and Type II errors for the maximum likelihood value (MLV), Kolmogorov-Smirnov (KS), and distance-to-nearest-neighbor (DTNN) tests. DTNN Type II errors can be reduced for the $N(0, 0, 1, 1, 0)$-vs-$N(0, 0, 0.25, 0.25, 0)$ test by imposing a two-dimensional linear cut on the distributions shown in Fig. 5. Such a cut was not used here because these values are for illustration only.

| Test                                      | CL    | Type II error | Comment                      |
|-------------------------------------------|-------|---------------|------------------------------|
|                                           |       | MLV test      | DTNN test | KS test |                           |
| $N(0, 0, 1, 1, 0)$ vs uniform             | 95%   | 0.0%          | 27.2%    | 66.2%   | cutting on minimal distance for DTNN |
|                                           | 50%   | 0.0%          | 0.5%     | 20.4%   |                           |
| $N(0, 0, 1, 1, 0)$ vs $N(0, 0, 0.25, 0.25, 0)$ | 95%   | 0.8%          | 55.9%    | 93.7%   | cutting on maximal distance for DTNN |
|                                           | 50%   | 0.0%          | 6.7%     | 17.1%   |                           |
| $N(0, 0, 1, 1, 0)$ vs two narrow normal pdfs | 95%   | 100%          | 0.0%     | 100%    | cutting on maximal distance for DTNN |
|                                           | 50%   | 97.1%         | 0.0%     | 18.4%   |                           |
| uniform vs $N(0, 0, 1, 1, 0)$             | 95%   | N/A           | 0.6%     | 75.6%   | cutting on maximal distance for DTNN |
|                                           | 50%   | 0.0%          | 0.1%     |         |                           |
Signal yields in this analysis are obtained using unbinned maximum likelihood fits to two-dimensional distributions of energy versus mass shown in Fig. 7. The two-dimensional background is modeled by the pdf

\[ f(\Delta E, m_{ES}) = A \cdot \exp(s \Delta E) \cdot m_{ES} \sqrt{1 - \frac{m_{ES}^2}{E_b^2}} \cdot \exp \left[ -\xi \left( 1 - \frac{m_{ES}^2}{E_b^2} \right) \right], \tag{7} \]

where \( \Delta E = E_{Kl} - E_b \) is the difference between the energy of the \( B \) candidate and the beam energy, \( E_b = 5.29 \text{ GeV}/c^2 \); \( m_{ES} \) is the beam-constrained mass of the \( B \) candidate; \( s \) and \( \xi \) are shape parameters; and \( A \) is a factor needed for proper normalization of the pdf. The signal shape is modeled by a normal-like function whose specific analytic expression is not important for this exercise.

We ask the following question: How consistent are the observed data with the background pdf? In other words, we compute goodness-of-fit values assuming that all events come from the background. The background pdf (7) is smooth while a hypothetical signal is expected to manifest itself through accumulation of events in a small region of the two-dimensional plot. In this case, the alternative hypothesis can be reasonably stated as “presence of peaks in the data”. Presence of peaks in the data would result in a smaller minimal distance \( d_m^{(i)} \) to \( m \) nearest neighbors than the one expected from the smooth background pdf.

To estimate the goodness-of-fit, we transform the background pdf (7) to uniform using Eq. (2), generate 10,000 MC experiments and determine the goodness-of-fit as a fraction of these MC experiments where the minimal distance \( d_m^{(i)} \) to nearest neighbor is less than the one observed in the data. We conclude that the \( B^+ \to K^+ e^+ e^- \) and \( B^+ \to K^+ \mu^+ \mu^- \) data...
are consistent with the fit at the 51% and 80% level, respectively. At this point, there is no indication of any peaks in the data.

Now we repeat the exercise described in the previous paragraph for $d_i^{(m)}$, $m > 1$. Goodness-of-fit values are plotted versus $m$ for both $K\ell\ell$ modes in Fig. 8. For a cluster of size 12, we estimate that the $B^+ \to K^+e^+e^-$ data are consistent with the fit only at the 0.13% level. At the same time, the goodness-of-fit for the $B^+ \to K^+\mu^+\mu^-$ data does not depend dramatically on the cluster size. The lowest goodness-of-fit value of 6.8% for the $B^+ \to K^+\mu^+\mu^-$ data corresponds to the test with clusters of size 8.

We conclude that the $B^+ \to K^+e^+e^-$ data are inconsistent with the background density. Not surprisingly, the data cluster that gives the maximal deviation from the background pdf consists mostly of points located inside the signal region.

6. SUMMARY

We have proposed a new method for estimation of goodness-of-fit in multidimensional analysis using a distance-to-nearest-neighbor test of uniformity. This procedure is recommended as a more versatile tool than the maximum likelihood methods for a vague generic alternative hypothesis. However, if the alternative hypothesis is stated in more specific terms, other methods may be superior.
FIG. 6: Maximal vs minimal distance to nearest neighbor computed under the uniform null hypothesis for the uniform pdf defined on a square $-5 \leq x \leq 5; -5 \leq y \leq 5$ and $\mathcal{N}(0, 0, 1, 1, 0)$.

FIG. 7: Difference $\Delta E$ (GeV) between the energy of the reconstructed $B$ candidate and the beam energy versus beam-constrained mass $m_{ES}$ (GeV/$c^2$) of the reconstructed $B$ candidate. Data for the $B^+ \rightarrow K^+e^+e^-$ decay are shown on the left, and data for the $B^+ \rightarrow K^+\mu^+\mu^-$ decay are shown on the right. Signal regions are shown with boxes. Data clusters that give maximal deviations from the expected pdf’s are shown with open circles.
FIG. 8: Goodness-of-fit (%) versus number of nearest neighbors (cluster size minus one) included in the goodness-of-fit calculation for the $B^+ \rightarrow K^+ e^+ e^-$ data (left) and $B^+ \rightarrow K^+ \mu^+ \mu^-$ data (right).

Acknowledgments

Thanks to Frank Porter for reviewing this note. Thanks to Art Snyder and Mike Sokoloff for comments. Thanks to Anders Ryd for providing details of the $B \rightarrow Kll$ analysis.
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