

Experiences from Tevatron Searches

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Abstract

In preparation for the possibility of new physics at the Large Hadron Collider at CERN, experiences gained at the Fermilab Tevatron collider experiments can be a useful guide for potential problems. This paper presents a review of recent applied statistical techniques and the problems for which they were required.

1 Introduction

The two Fermilab Tevatron collider experiments, CDF and DØ, both probe a broad range of elementary particle physics. Of particular interest are searches for new particles or evidence for new physics. It is anticipated that the new energy frontier at the Large Hadron Collider (LHC) at CERN will create opportunities for observing new physics beyond the electroweak scale. Experiences from searches for new physics at the Tevatron should provide insight into the problems that LHC experiments will likely face. This paper presents a brief review of the problems addressed by several modern Tevatron searches.

Many searches at the Tevatron result in a relatively unambiguous statistical significance. Two excellent examples of this are the direct observation of the Ξ_b^\pm baryon at DØ [1] and the observation of orbitally excited B_s^{**} mesons [2]. Figure 1 shows the reconstructed mass of the Ξ_b^\pm baryon and Fig. 2 shows the mass difference in candidates for orbitally excited B_s^{**} decays. Although both are exciting examples of discovery, these searches do not represent challenges or ambiguity in the estimation of search significance. Most of the problems for Tevatron searches arise from the convergence of small signal rates, large background rates, and large relative uncertainties on nuisance parameters inherent to the search. It is these cases which will be the focus of this paper.

2 Systematic Uncertainties

In many searches for small signals, a significant limiting factor is the relative size and nature of systematic uncertainties on the measurement of background processes. In the large-statistics limit of a search, a precise knowledge of systematic uncertainties is required to reliably determine search significance. In

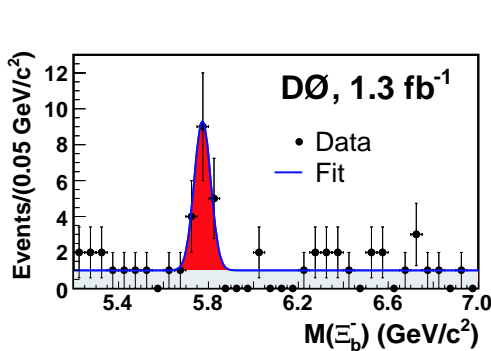


Fig. 1: The background-subtracted invariant mass of Ξ_b^\pm baryons at the DØ experiment.

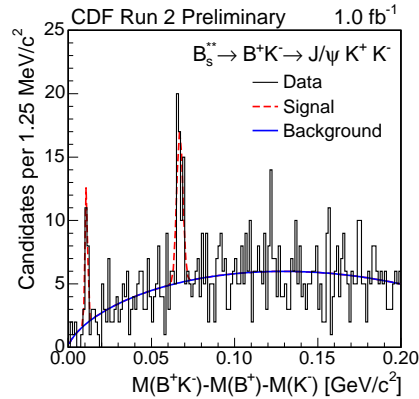


Fig. 2: The mass difference in candidates for orbitally excited B_s^{**} decays at the CDF experiment.

searches for small signals at the Tevatron, the uncertainty on the background rate is often over an order of magnitude larger than the signal rate itself, and is thus a dominant factor in signal sensitivity. There are two broad classes of such uncertainties:

- Type I: Uncertainties related to gross normalizations or rates of acceptance. These are generally constrainable by control samples and the relative size scales according to the statistics of the control samples.
- Type II: Uncertainties related to the understanding of the features of data measurements and experimental resolutions. These often manifest as uncertainties on the shapes of differential distributions involved in event selection procedures.

Type I uncertainties are generally assumed to arise from parent distributions which are Gaussian in nature. Errors in the estimation of background process rates occur when these uncertainties are actually non-Gaussian or asymmetric. Estimates of Type I uncertainties must also be sensitive to regions of truncation which occur, for example, when efficiencies reach either 0% or 100%. Type II uncertainties can present a significant challenge when their impact to an event selection is difficult to properly measure. The size of these uncertainties are often inflated to partially accommodate this difficulty, which in turn degrades search sensitivity. A worrying scenario arises when Type II uncertainties are not propagated through high-dimension multivariate analyses, thus incorrectly overestimating signal significance. A careful understanding of systematic uncertainties is considered a prerequisite to performing a detailed statistical analysis for a search.

The finite statistics of simulated samples used to predict the rates of different classes of events represents a particular challenge in searches for small signals. In many cases, the uncertainty on the shape of a differential distribution or multivariate analysis discriminant is dominated by the statistical uncertainty on the prediction. A common solution is to use a smoothing algorithm to make an estimate of the true parent distribution. There are two smoothing techniques used frequently at the Tevatron: the 353QH algorithm [3] which is implemented in the ROOT software package [4] and Gaussian kernel estimation [5]. A more complete comparison of the two algorithms is presented in [5]. As an alternative to smoothing, the true shape of the parent distribution of a statistics-limited sample can be estimated from the shape of the same variable at a less restricted point in the selection process. For example, an analysis that selects two quark-jets and requires that both jets be tagged by a b-quark identification algorithm could model the shape of the double b-tagged distribution by the shape of the less restrictive single b-tagged selection. After a proper normalization, the remaining biases of the b-tagging algorithm are often smaller and better understood than the uncertainty on the statistics-limited shape of the double-tagged sample. This method is often used in conjunction with a smoothing algorithm, but is sensitive to the nature of the intermediate selection used.

3 The Tevatron Higgs Search

The search for a standard model (SM) Higgs boson at the Tevatron provides a good example of the implementation of several statistical techniques used in searches for small signals. The statistical analysis begins with an assumption of two hypotheses which are to be tested:

- Null hypothesis (**H0**): A compound hypothesis with an associated set of nuisance parameters each with its own uncertainty. This hypothesis can be considered to be the background-only hypothesis.
- Test hypothesis (**H1**): The test hypothesis is the same as **H0**, but a signal for new physics is added. Thus, **H1** adopts the necessary signal model parameters and possibly additional nuisance parameters.

In this example, **H0** describes the SM background expectation for the results of a Higgs search and is the sum of several contributing physical processes. The nuisance parameters are the luminosity

normalization, acceptance, background cross sections, etc. The test hypothesis adds the SM Higgs signal and is parameterized by Higgs mass, production cross section, and decay branching fractions. Both **H0** and **H1** are subdivided according to final states with unique signatures. These final states are orthogonal search channels defined to maximize acceptance and to isolate regions with high signal significance. At the Tevatron, two different statistical analysis treatments are utilized: a Bayesian integration [6] and the semi-Frequentist CL_S method [7]. More detailed references for the Tevatron SM Higgs searches can be found here [8, 9].

3.1 The Bayesian Treatment

The Bayesian approach utilized in the Tevatron Higgs search begins by assuming a Poisson-distributed probability distribution for the observed numbers of events selected. The posterior probability density function (PDF) for a set of signal and background model parameters θ_R is given by:

$$p(\theta_R|\vec{x}) = \frac{\int L(\vec{x}|\theta_R, \theta_S) \pi(\theta_R, \theta_S) d\theta_S}{\int \int_{-\infty}^{\theta_{Rcut}} L(\vec{x}|\theta_R, \theta_S) \pi(\theta_R, \theta_S) d\theta_S d\theta_R} \quad (1)$$

where $\pi(\theta_R, \theta_S)$ is the prior probability density for θ_R and the set of nuisance parameters θ_S . The likelihood $L(\vec{x}|\theta_R, \theta_S)$ is the joint probability density over all analysis channels and bins of the final variables and the observed data \vec{x} . The parameter θ_{Rcut} is chosen to ensure unitarity, and for an appropriately chosen prior can generally be infinity. The most common choices for prior probability density for the signal is the Heaviside unit step function, and the prior for all nuisance parameters is taken as Gaussian. The limit on the rate of signal events is then determined by integrating the posterior density function to the desired fraction of the total integral, β :

$$\beta = \int_{-\infty}^{\theta_{R\beta}} p(\theta_R|x) d\theta_R \quad (2)$$

which defines $\theta_{R\beta}$ as the limit on the model parameter at a Bayesian confidence level of β .

3.2 The CL_S Treatment

The semi-Frequentist CL_S approach also assumes Poisson-distributed sources of events and begins by constructing a joint likelihood ratio test statistic:

$$Q = -2 \text{Log} \frac{L(\vec{x}|\theta_{R1}, \hat{\theta}_S)}{L(\vec{x}|\theta_{R0}, \hat{\theta}_S)} \quad (3)$$

where the profile likelihood $L(\vec{x}|\theta_{R1}, \hat{\theta}_S)$ is the Poisson likelihood for the physics parameters of **H1** and the set of nuisance parameters which maximize the likelihood for **H1** ($\hat{\theta}_S$). Likewise, $L(\vec{x}|\theta_{R0}, \hat{\theta}_S)$ represents a maximization for the physics parameters of **H0**. This test statistic is used to describe the outcomes of multiple repetitions of the experiment for which pseudo-experiment trials are drawn from Poisson-distributed outcomes of the **H0** and **H1** hypotheses. The uncertainties on the N nuisance parameters for each source of events are assumed to have a Gaussian PDF. For each pseudo-experiment, the mean value for the expected number of signal and background events is randomly drawn from an N -dimensional Gaussian distribution, described by the N nuisance parameters and their uncertainties.

The PDFs for the test statistics of **H0** and **H1** are then used to evaluate confidence intervals of the following definition:

$$CL_S = 1 - \frac{CL_{S+B}}{CL_B} \quad (4)$$

where the confidence levels CL_{S+B} and CL_B are defined by integrating the corresponding PDFs from the observed test statistic to infinity. An exclusion of a signal model parameter (parameterized as F) at a confidence level of α is achieved when the model parameter satisfies $\alpha \leq 1 - \frac{CL_{S+B}(F)}{CL_B(F)}$.

3.3 Drawbacks of Methodology

Practically speaking, statistical treatments with discrete numbers of events lead to imperfect coverage for any method. This unavoidable consequence demands a conservative treatment to ensure well-understood coverage. The Bayesian treatment suffers from both larger issues with coverage but also the choice of prior. While priors are somewhat unpopular in the field of particle physics due to potential biases, a careful choice of prior can generally construct a test with the desired properties. It is generally accepted that the CL_S method is a less rigorous means of communicating exclusions of signal hypotheses. However, the properties of the CL_S test appear to be robust for this purpose. The formulation of the test has the agreeable feature of giving a conservative response for exclusion in insensitive signal regions. The approach chosen at the Tevatron is to maintain both treatments in as many cases as possible. This serves both as a cross check of results, but can also lead to insight in the fundamental behavior of small signal searches.

4 The Tevatron Search for Single Top Quark Production

In 2007, the DØ collaboration announced it had observed first evidence for the electroweak production of single top quarks [10]. At the same time, the CDF collaboration announced that with analyses of similar sensitivity it did not find the same results [11, 12, 13]. This scenario may occur between the LHC experiments and the treatment at the Tevatron therefore has pedagogical value. Adopting the nomenclature from the previous section, the descriptions of the **H0** and **H1** hypotheses are identical for the Tevatron search for single top quarks aside from the parameterization of the signal.

4.1 The DØ Single Top Search

The DØ measurement was constructed using a Bayesian calculation similar that defined in Eqn. 1. Three semi-independent analyses observed an excess of events consistent with single top quark production near the expected SM rate of 2.9 pb. The measurement of the observed cross section was based on a binned likelihood derived from the analysis discriminants:

$$y = a\sigma + \sum_{s=1}^{N_{bkgd}} b_s \quad (5)$$

$$P(D|y) = P(D|\sigma, a, b) = \prod_{i=1}^{N_{bins}} P(D_i|y_i) \quad (6)$$

where the index s runs over the number of background sources in **H0**. The Bayesian posterior PDF was calculated as a function of cross section, assuming a Heaviside unit step function prior density probability. As demonstrated in Fig. 3, the measured signal cross section is determined from the peak of the posterior PDF and the uncertainty is taken from the width near the peak. Figure 4 shows the actual measurement derived from one of the three analysis techniques.

The estimates of search sensitivity and the significance of the observed result were described using p-values derived from pseudo-experiments. For each pseudo-experiment, the values of the nuisance parameters were sampled from Gaussian PDFs. The p-values were reported with the following definitions:

- Expected p-value: The fraction of **H0** pseudo-experiments measuring at least the SM single top quark cross section of 2.9 pb.

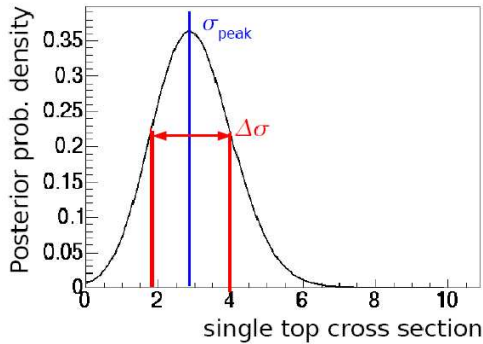


Fig. 3: An example of the Bayesian posterior density distribution for pseudo-experiments with a single top quark signal with the SM rate of 2.9 pb for the $D\bar{0}$ experiment.

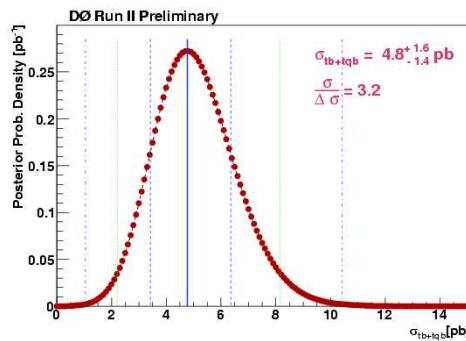


Fig. 4: The Bayesian posterior density distribution for pseudo-experiments derived from the observed data distribution for the $D\bar{0}$ experiment.

Table 1: DZero ST Data

	Expected p-value	Observed p-value	SM p-value	Observed Cross Section
Analysis 1	0.019 (2.1σ)	0.00035 (3.4σ)	0.11 (1.2σ)	4.9 pb
Analysis 2	0.037 (1.8σ)	0.0021 (2.9σ)	0.21 (0.8σ)	4.6 pb
Analysis 3	0.097 (1.3σ)	0.0089 (2.4σ)	0.175 (0.9σ)	5.0 pb

Table 2: DZ ST Cov Matrix

Analysis 1	1.0	0.57	0.51
Analysis 3	-	1.0	0.45
Analysis 2	-	-	1.0
Weight	0.401	0.452	0.146

- Observed p-value: The fraction of H_0 pseudo-experiments measuring at least the observed cross section.
- SM p-value: The fraction of H_1 pseudo-experiments measuring at least the observed cross section.

The results of these measurements along with the observed cross section for each analysis are given in Table 1. The results seem to indicate an upward fluctuation in the data rate, but are demonstrably more compatible with the H_1 hypothesis.

Given three highly correlated analyses, the $D\bar{0}$ researchers employed the Best Linear Unbiased Estimate (BLUE) technique [14] to combine the measurements and determine a more sensitive estimate of the observed signal significance. The BLUE technique essentially describes a linear function of weighted measurements. The weights are determined by inverting the correlation matrix for the system of measurements. The covariance matrix obtained via pseudo-experiments and the corresponding linear weights for the $D\bar{0}$ analyses are shown in Table 2. Using this linear combination, a new set of pseudo-experiments was generated to determine the observed signal significance. Via this technique, the original best value of 4.9 ± 1.4 pb was refined to 4.8 ± 1.3 pb, reported as 3.5 standard deviations, and more recently as 4.7 ± 1.3 pb [15].

4.2 The CDF Single Top Search

The CDF collaboration performed a similar search for single top quark production in an equal-sized data sample. Using a similar analysis approach, CDF researchers applied three different multivariate analyses

Table 3: CDF ST Data

	Exp. p-value	Obs. p-value	Exp. CL_S	Obs. CL_S	Exp. Limit	Obs. Limit
Analysis 1	0.005 (2.6σ)	0.525 (-)	-	-	2.9 pb	2.6 pb
Analysis 2	0.025 (2.0σ)	0.585 (-)	0.05	0.039	2.9 pb	2.7 pb
Analysis 3	0.006 (2.5σ)	0.01 (2.3σ)	-	-	-	-

Table 4: CDF ST Cov Matrix

Analysis 1	1.0	0.59	0.70
Analysis 3	-	1.0	0.65
Analysis 2	-	-	1.0

to estimate significance. However, the expected and observed significance of each analysis was reported in a slightly different manner. As in the case of the $D\bar{D}$ statistical analyses, the values of the nuisance parameters used in pseudo-experiments are drawn from Gaussian PDFs:

- Analysis 1:
 - Expected p-value: The fraction of H_0 pseudo-experiments measuring at least the SM single top quark cross section of 2.9 pb.
 - Observed p-value: The fraction of H_0 pseudo-experiments measuring at least the observed cross section.
- Analysis 2: The same p-values reported by Analysis 1 were given, and the CL_S confidence level (Eqn. 4) was also reported.
- Analysis 3: The same p-values reported by Analysis 1 were given, and the Bayesian calculation described in the Sec. 4.1 was used to measure an observed cross section.

The analysis results were mixed, with two analyses excluding single top quark production above 2.6 pb and 2.7 pb respectively, while the third analysis observed a 2.3σ effect at 2.7 ± 1.2 pb. All three analyses had a similar expected sensitivity and used the same data, reconstruction, and Monte Carlo simulation. To understand the compatibility of the three measurements, the CDF researchers also utilized the BLUE technique. The covariance matrix for the CDF analyses is given in Table 4. With the linearly-combined estimator, a combined measurement was evaluated and a χ^2 value for each pseudo-experiment was determined. An estimate of analysis compatibility was determined by measuring the fraction of pseudo-experiments whose χ^2 value exceed the value observed data. This fraction was found to be 0.65%.

4.3 Comparison of Results

Both Tevatron experiments devised multiple analyses, all with similar search sensitivities in the same size data sample. The agreement of results amongst the three $D\bar{D}$ analyses is not unexpected considering the design of the analyses, and the additional search sensitivity gained via the linear combination of results is indeed small. The conflicting results from the CDF analyses is perhaps more interesting. It is conceivable that the results reflect internal biases within the analyses. It is also possible that the analyzers were unlucky, to use the particle physics jargon, and the data reflected a downward fluctuation of stochastic processes. At the time of this publication, the $D\bar{D}$ researchers have updated two of their analysis techniques and found similar results [15]. At this time, there is no public update of the CDF single top quark search.

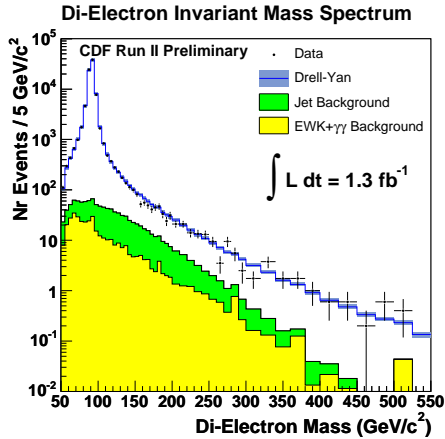


Fig. 5: The di-electron invariant mass spectrum from the CDF experiment.

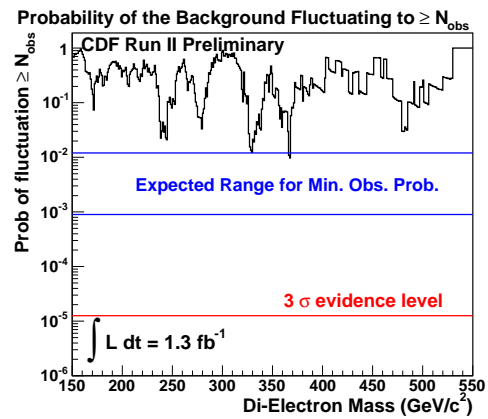


Fig. 6: The Poisson probability for data as a function of di-electron mass.

5 Model Independent Searches

The previous two examples of the standard model Higgs boson search and the single top quark search exemplified directed searches for new physics at the Tevatron. Each uses very modern approaches to analysis and statistical interpretation, but are inherently linked to assumptions which impact the interpretation of the results. As an alternative, a second class of searches removes all model parameters for new physics from the analysis design and allows them to be introduced after a statistical interpretation of the results has been performed. There are two general categories for such searches: bump hunts and broad spectrum searches.

5.1 Bump Hunts

Given a well-understood differential distribution, researchers can search for deviations from nominal predictions of the shape and rate of that distribution. As an example, we will consider the model-independent search for a high-mass resonance in the di-electron mass spectrum at the CDF experiment. The di-electron mass spectrum is well-studied at the Tevatron as the global energy-scale calibration procedure for both experiments relies upon accurate knowledge of Drell-Yan Z boson production and high-resolution detection of electrons. Figure 5 contains an example of the CDF di-electron mass spectrum corresponding to 1.3 fb^{-1} of data [16].

The analysis of the di-electron mass spectrum proceeded by using a variable-sized sliding window of the form $W(M_{ee}) = 4.8 + 0.044 \times M_{ee}$ with a step size of $1 \text{ GeV}/c^2$. For each step, the significance of any excess above the SM prediction was evaluated via a Frequentist p-value. Assuming Poisson-distributed background rates and Gaussian uncertainties on the rates of backgrounds, the p-value is defined as the fraction of background-only pseudo-experiments which equal or exceed the number of events observed in the window. The results of this test are shown in Figure 6 as a function of the di-electron mass. The authors define an expected range for minimum observation probability of 5%-0.27% region as the expected range to find the minimum Frequentist p-value over the tested mass range [16]. The minimum p-value for the spectrum is 9.7×10^{-3} with the sliding window centered at $M_{ee} = 367 \text{ GeV}/c^2$.

Such a search is certainly hampered the lack of a signal model, but presents a broad application for theoretical model interpretation. As such, this technique is a valuable approach to studying the gross features of a data sample. The analyzers went on to interpret the search using both a set of Z' models and Randall-Sundrum graviton models, each resulting in a more sensitive probe to the specified new physics model than the model-independent search.

5.2 Broad Spectrum Searches

The range of physics processes at the Tevatron and LHC contains a rich phenomenology of search possibilities. Despite being an exciting opportunity for the observation of new physics, there are several challenges which must be faced. First, limited human and computing resources force the prioritization of search design and implementation. Second, a comparison and correlation of search results in a broad range of final states is often made opaque by differing search techniques and interpretations. The Tevatron has seen the development of a few broad spectrum search techniques which attempt to address these problems, amongst others. As an example, we present the two most modern versions implemented at the CDF experiment: Vista and Sleuth.

The Vista program [17] searches for large cross-section physics in final states with high- p_T (high transverse momentum) physics objects. The basic algorithm proceeds as follows:

1. Select high- p_T ($p_T > 17\text{GeV}/c$) electrons, photons, muons, tau-leptons, hadronic jets, and neutrinos (manifested as missing transverse energy) which pass the detector's physics triggers.
2. Events are passed through an offline filter to isolate interesting final states.
3. Standard model background simulations are generated and the detector response is simulated.
4. Orthogonal subsets of events are formed and kinematic distributions are populated.

The current implementation of Vista identifies a total of 344 final states and 16486 kinematic distributions. The program forms a global χ^2 for a comparison of the simulation to data and minimizes it over 44 total nuisance parameters, 26 of which are externally constrained. Following this minimization, the total numbers of events are compared for each final state and each kinematic distribution is evaluated using the Kolmogorov-Smirnov statistic. An example of a discrepant distribution identified by the Vista program is shown in Fig. 7.

The Sleuth program [18] is a quasi-model-independent tool used to search for new physics in high- p_T final states. To be sensitive to electroweak-scale new physics, the program analyses the tails of the summed transverse momentum ($\sum p_T$). The program interfaces with the Vista program by adopting its orthogonal set of final states and its comprehensive correction model. The statistical test for each final state in the Sleuth program is as follows:

1. Identify D regions in D data points defined by the semi-infinite integral of the $\sum p_T$ kinematic distribution.
2. Define the interestingness (\mathcal{P}_N) of a region containing N data points as the Poisson probability the SM prediction would fluctuate up to or above N .
3. The most interesting region (\mathcal{R}) is found by minimizing \mathcal{P}_N for the final state.
4. Pseudo-experiments of the SM $\sum p_T$ distribution are used to generate a population of \mathcal{P}_N associated with the value \mathcal{R} for each final state.
5. The fraction of regions more interesting than \mathcal{R}_{obs} quantifies each final state.

Considering all final states, the program determines the most interesting region \mathcal{R}_{max} . Using this region, the statistic $\tilde{\mathcal{P}}$ is defined as the fraction of pseudo-experiments that would generate a region in any final state more interesting than \mathcal{R}_{max} , including a proper accounting for the number of final states considered. Assuming that the simulation and correction model are accurate, the distribution of $\tilde{\mathcal{P}}$ in all final states should be uniform in the range $0 \rightarrow 1$. In the presence of an unmodeled source of physics, the value of $\tilde{\mathcal{P}}$ should be small.

In 927 pb^{-1} of data at the CDF experiment, the Sleuth program found $\tilde{\mathcal{P}} = 0.46$. The Sleuth program would interpret this as no indication for new physics in the distributions it probes, while the threshold for the pursuit of potential discovery is chosen by the authors at $\tilde{\mathcal{P}} < 0.001$. The most interesting final state in this data sample as identified by the Sleuth program is the two b -quark final state, as

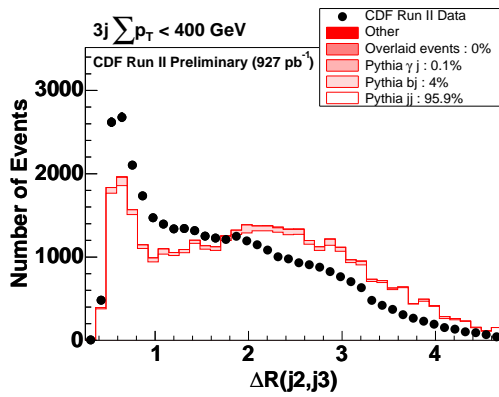


Fig. 7: One of the most discrepant kinematic distributions identified by the Vista program at the CDF experiment.

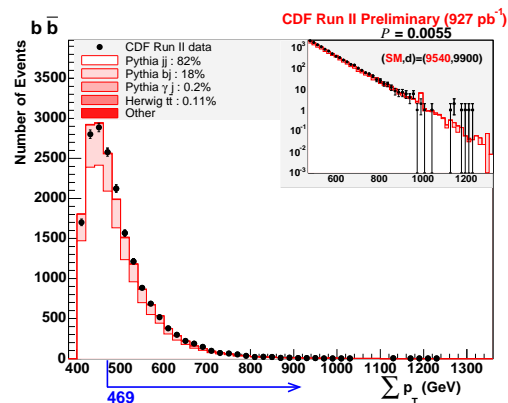


Fig. 8: The most discrepant summed p_T distribution found by the Sleuth program at the CDF experiment.

shown in Fig. 8. It should be noted that this tool is not intended to be a bypass for directed searches, but rather an effective means for evaluating an experiment's data in a systematic manner.

6 Summary

The statistical techniques employed in recent Tevatron searches encompass a broad range of interpretation and utility. The transition to the new energy frontier at the CERN LHC will indeed be exciting and is eagerly anticipated by many. It is expected that the LHC experiments will face similar challenges in searches for new physics as those seen at the Tevatron. The experiences from Tevatron searches will hopefully be both useful and instructive for probing the data at the LHC.

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