Heavy flavour jet abundances and tagging rates analytically determined

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Abstract. Heavy flavour jet tagging is widely used in the determination of cross sections including the production of heavy flavoured quarks. This requires the knowledge of heavy and light flavour jet tagging efficiencies and their uncertainties. A system of eight non-linear equations can be used to determine these quantities by means of two different tagging algorithms and two data sets which differ in heavy flavour jet content. The analytical solution of this system of equations, derived by means of resultants is described in detail, including a discussion about its singularities which provide important insights, such as prescriptions to prevent badly chosen sample flavour compositions and working points of the used tagging algorithms. The analytical solution also provides an efficient and transparent way to determine the uncertainties on the solved quantities, taking correlations into account.

Heavy flavour jets, Tagging

PACS numbers: 14.65.Fy, 14.65.Bt, 21.10.Tg

1. Introduction

Heavy flavour jet tagging is widely used in the determination of cross sections including the production of heavy flavoured quarks. This encompasses interesting physics processes, such as top anti-top quark pair production, $Z \rightarrow b\bar{b}$ production, Higgs boson production ($H \rightarrow b\bar{b}$), etc. The $b$ quarks fragment into long-lived hadrons, whose decay products manifest typically in the tracking system of a detector as displaced charged particle tracks. The energy deposits of particles are measured in the calorimeter of the detector. They are used to reconstruct jets, to which charged tracks can be associated.

In simulation one can easily identify the quark flavour of a jet by checking if a heavy flavour quark or hadron is geometrically located inside the jet. In data one has to rely on reconstructed objects and quantities such as associated track displacements to determine the flavour content of a jet. Dedicated algorithms - referred to as tagging algorithms - have been developed to determine the flavour of jets based on their lifetime information. This procedure is not perfect and implies certain probabilities for the correct identification of jet flavours. The uncertainties on these probabilities enter among others into the systematics of cross section measurements of the physics processes...
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It is indispensable to determine the heavy and light flavour jet tagging efficiencies and their uncertainties as accurate as possible.

System8 \cite{1} provides an Ansatz which allows one to determine these quantities. It consists of a system of eight algebraic equations

\begin{align}
  n &= n_b + n_q, \\
  n_T &= \varepsilon_T n_b + f_T n_q, \\
  n_S &= \varepsilon_S n_b + f_S n_q, \\
  n_{TS} &= \varepsilon_T \varepsilon_S n_b + f_T f_S n_q, \\
  p &= p_b + p_q, \\
  p_T &= \varepsilon_T p_b + f_T p_q, \\
  p_S &= \varepsilon_S p_b + f_S p_q, \\
  p_{TS} &= \varepsilon_T \varepsilon_S p_b + f_T f_S p_q,
\end{align}

where \( n \) is a data sample of a given number of jets. It consists of two subsamples, one containing the number of heavy flavour jets \( n_b \) and another one containing the number of light flavour jets \( n_q \). The contribution of charm flavoured jets is predominantly absorbed into the light flavour subsample. Similarly, another data sample \( p \) can be subdivided in its heavy and light flavour contributions \( p_b \) and \( p_q \). It is important that the two data samples \( n \) and \( p \) differ in their flavour composition; otherwise the system of eight equations degenerates to a system of four linearly independent equations which cannot be solved for its eight unknowns anymore. The two data samples can share common jets and are therefore in general not statistically independent. The efficiencies to tag heavy flavour jets are designated as \( \varepsilon \) and the efficiencies to tag light flavour jets - also referred to as fake rates - are designated with \( f \). To determine these efficiencies and fake rates, two different tagging algorithms \( T \) and \( S \), which have to be de-correlated \cite{2}, are needed.

The de-correlation requirement can be achieved in choosing two tagging algorithms \( T \) and \( S \), which determine the flavour based on the information of different jet or associated track quantities which are de-correlated. In practice one tagging algorithm can be chosen, based on the lifetime information of a jet through the impact parameter of associated tracks, e.g. by means of a secondary vertex \cite{3} \cite{4} tagger. Since muons in jets are a signature of heavy flavour decay an appropriate choice for the second tagging algorithm is a muon tagger, which looks for muons in jets with a certain transverse momentum with respect to the jet axis. In the following, it is assumed that the taggers are fully de-correlated, in which case the unknown quantities can be obtained relying on data only. Otherwise, correlation factors determined by simulation have to be introduced into the system of eqs. \cite{1}.

The known quantities that appear in the system of equations (the number of jets in each of the two samples before and after one or both taggers have been applied) are on the left hand side of eqs. \cite{1}. The eight unknown quantities, which are the heavy
and light flavour jet content of the samples and the tagging efficiencies and fake rates, appear on the right hand side.

The analytical solution of the system of equations will be derived in the next section, followed by a discussion of its numerical stability and the determination of errors on the solved quantities in section 3. An explicit example, showing the performance of the method is given in section 4.

2. Analytical solution

Elementary algebraic operations permit one to reduce the system of eight equations to two equations of two unknowns, which are polynomials of multi-degree two. The choice of the two unknowns is not unique. Since the primary goal is to determine the heavy flavour jet tagging efficiency and the fake rate of a tagging algorithm $T$ to be used in various data analyses, it is convenient to keep the two unknowns $\epsilon_T$ and $f_T$ in the two polynomials. The other unknowns can be obtained by backward substitution. In general two multi-variate polynomials of two unknowns with arbitrary degree can be solved by means of resultants [5] [6]. The two polynomials can be written in the form

$$r_1 := a_0 f_T + a_1 = 0,$$
$$r_2 := b_0 f_T + b_1 = 0.\quad(2)$$

The coefficients $a_0$, $a_1$ and $b_0$, $b_1$ are polynomials in the unknown $\epsilon_T$. Their explicit expressions are given by

$$a_0 = a_{00} \epsilon_T + a_{01},$$
$$a_1 = a_{10} \epsilon_T + a_{11},$$
$$b_0 = b_{00} \epsilon_T + b_{01},$$
$$b_1 = b_{10} \epsilon_T + b_{11},\quad(3)$$

where the coefficients can be expressed in terms of the initial known quantities as

$$a_{00} = -n^2 p_S + n_S n p,$$
$$a_{01} = n n_T p_S - n_S n_T p,$$
$$a_{10} = a_{01},$$
$$a_{11} = n_T n_T S p - n_T S p_T n + n_S n_T p_T - n_T^2 p_S \quad(4)$$

for the first polynomial and

$$b_{00} = -n_S n_T p - p_T S n^2 + n_T S p n + n_S p_T n,$$
$$b_{01} = -n_T S p_T n + p_T S n n_T,$$
$$b_{10} = b_{01},$$
$$b_{11} = n_T S p_T n_T - p_T S n_T^2,\quad(5)$$

for the second polynomial. The resultant with respect to $f_T$ in eqn. 2 can then be obtained by equating the determinant of the Sylvester matrix [7]

$$Res(f_T) = \begin{vmatrix} a_0 & b_0 \\ a_1 & b_1 \end{vmatrix} \quad(6)$$
to zero. The solution is a univariate polynomial of degree two which can be solved for the first unknown
\[
\epsilon_T = -\frac{1}{2} a_{00} b_{11} - a_{11} b_{00} + \sqrt{\left(-\frac{1}{2} a_{00} b_{11} - a_{11} b_{00}\right)^2 - \frac{a_{01} b_{11} - a_{11} b_{01}}{a_{00} b_{10} - a_{10} b_{00}}}.
\] (7)

The solution has a two-fold ambiguity originating from the initial system of equations which is symmetric with respect to exchange of efficiencies and fake rates. In practice, the larger solution given above (positive square root) corresponds to the efficiency. The remaining unknowns can be obtained through backward substitution and are given by
\[
f_T = -\frac{a_1}{a_0} ,
\] (8)
\[
\epsilon_S = \frac{n_T S - n_S f_T}{n_T - f_T n} ,
\] (9)
\[
f_S = \frac{n_S (\epsilon_T - f_T) + \epsilon_S (f_T n - n_T)}{n \epsilon_T - n_T} ,
\] (10)
\[
n_b = \frac{n_T - f_T n}{\epsilon_T - f_T} ,
\] (11)
\[
n_q = n - n_b ,
\] (12)
\[
p_b = \frac{p_T - f_T p}{\epsilon_T - f_T} ,
\] (13)
and
\[
p_q = p - p_b .
\] (14)

In the more general case where arbitrary correlation factors are taken into account in the system of equations some terms do not cancel out each other and the resultant yields a univariate polynomial of degree eight, which cannot be solved analytically anymore (though it could be solved semi-analytical by means of Sturm’s theorem which gives the number of real roots of a given univariate polynomial of arbitrary degree in a given interval [5]. The roots would need to be polished e.g. by binary bracketing and one would need to take care about the increased number of solution ambiguities).

3. Numerical stability and error propagation

The solution of the initial system of eight equations contains three singularities due to vanishing denominators in case of not carefully chosen working points. A first singularity occurs in the denominator of eqn. 9 which determines the efficiency \( \epsilon_S \). The singularity of the type \( (n_T - n f_T) \) appears if all tagged jets are of light flavour and they have been misidentified as heavy flavour jets. This would certainly correspond to an ill-posed initial condition which prohibits the sensible use of a given tagging algorithm. The second singularity occurs in the denominator of eqn. 10 which determines the fake rate \( f_S \). A singularity of type \( (n_T - n \epsilon_T) \) appears if all tagged jets are of heavy flavour.
This particular case corresponds to a perfect algorithm which could be solved with just four equations. In practice it cannot be avoided that some of the tagged jets will be misidentified. The fake rate of optimised tagging algorithms depends on the working point, which is typically chosen at the percent level (see e.g. [8]) far away from zero within real precision at which point the implementation of the analytical solution looses its power of prediction. The last singularity occurs in the denominator of eqs. [11] and [13]. There, the singularity of type \((\epsilon_T - f_T)\) corresponds to the case of equal efficiency and fake rate. The efficiency and fake rate of a given tagging algorithm could be determined with a system of four equations but one would not be able to determine the heavy and light flavour content of the sample. This working point is far away from typical chosen settings which are driven by the goal of having a maximal efficiency at minimal fake rate. To prevent the problematic regions around the singularities one has to choose working points of the taggers which avoid small or even vanishing denominators. This can be achieved in probing different working points and verifying the values of the denominators.

The errors of the analytical solution are obtained through gaussian error propagation taking all correlations into account. The evaluation of the errors of subsequently solved quantities, obtained through backward substitution, is accurately done by error propagation through differentials as explained below. In this way the errors of the subsequent solved quantities conserve all their dependencies on the knowns such that terms with different signs compensate before the gaussian quadrature takes place.

The errors of the knowns entering into the error propagation are the errors of the data samples \(n\) and \(p\), which are assumed to be Poisson distributed. The errors of the tagged subsamples \((n_T, p_T, n_S, p_S, nTS\) and \(pTS\)) are taken binomial since the subsamples have been obtained by applying a binary acceptance/rejection procedure through the taggers. They can be computed from the known variables as

\[
\begin{align*}
\Delta n &= \sqrt{n}, \\
\Delta n_T &= \sqrt{n_T(n - n_T)/n}, \\
\Delta n_S &= \sqrt{n_S(n - n_S)/n}, \\
\Delta n_{TS} &= \sqrt{n_{TS}(n - n_{TS})/n} \\
\end{align*}
\]

and equivalently for the data sample \(p\). The variance of the tagging efficiency is then given by

\[
(\Delta \epsilon_T)^2 = \left(\frac{d\epsilon_T}{dn}\right)^2 (\Delta n)^2 + \left(\frac{d\epsilon_T}{dp}\right)^2 (\Delta p)^2 + \left(\frac{d\epsilon_T}{dn_T}\right)^2 (\Delta n_T)^2 + (\frac{d\epsilon_T}{dn_T}) (\Delta n_T) (\Delta \epsilon_T)

+ \left(\frac{d\epsilon_T}{dp_T}\right)^2 (\Delta p_T)^2 + \left(\frac{d\epsilon_T}{dn_S}\right)^2 (\Delta n_S)^2 + \left(\frac{d\epsilon_T}{dp_S}\right)^2 (\Delta p_S)^2

+ \left(\frac{d\epsilon_T}{dn_{TS}}\right)^2 (\Delta n_{TS})^2 + \left(\frac{d\epsilon_T}{dp_{TS}}\right)^2 (\Delta p_{TS})^2 + 2 \frac{d\epsilon_T}{dn} \frac{d\epsilon_T}{dp} \epsilon_{np} \Delta n \Delta p
\]
\[
\frac{d\xi_T}{dn} \frac{d\xi_T}{dp_T} \Delta n \Delta p_T + \frac{d\xi_T}{dn} \frac{d\xi_T}{dp_s} \Delta n \Delta p_s
\] + \frac{d\xi_T}{dn} \frac{d\xi_T}{dp_{TS}} \Delta n \Delta p_{TS} + \frac{d\xi_T}{dn_T} \frac{d\xi_T}{dp_{TP}} \Delta n_T \Delta p_T
\] + \frac{d\xi_T}{dn_T} \frac{d\xi_T}{dp_{TPS}} \Delta n_T \Delta p_{TPS} + \frac{d\xi_T}{dn_T} \frac{d\xi_T}{dp_s} \Delta n_T \Delta p_T
\] + \frac{d\xi_T}{dn} \frac{d\xi_T}{dp_{TS}} \Delta n \Delta p_{TS} + \frac{d\xi_T}{dn_T} \frac{d\xi_T}{dp_{TS}} \Delta n_T \Delta p_{TS}
\] + \frac{d\xi_T}{dn_T} \frac{d\xi_T}{dp_{TS}} \Delta n_T \Delta p_{TPS} + \frac{d\xi_T}{dn_T} \frac{d\xi_T}{dp_{TPS}} \Delta n_T \Delta p_{TPS}
\] and equivalently for the fake rate \( f_T \) and the other solved quantities. The correlation coefficient \( \varrho \) of two variables \( n_a \) and \( p_b \) can be determined by means of the relation
\[
\varrho_{n_a p_b} = \frac{1}{n \cup p} (n_a \cap p_b - \frac{n_a p_b}{n \cup p}) \quad (16)
\]
where \( n \cup p \) are the jets belonging to the sample \( n \) or \( p \) and \( n_a \cap p_b \) are the jets in common between the subsamples \( n_a \) and \( n_b \). It should be noted that the total number of jets per event could also be exploited in the definition of the correlation coefficient. Given the fact that the correlation terms are in general small the definition above is used in the following without further discussion. To keep the numerical evaluation efficient, the derivatives are computed exploiting differentials \( (d\xi_T, df_T, d\xi_S, df_S, dn_b, dn_q, dp_b, dp_q) \). The derivative of the tagging efficiency with respect to the data sample size \( n \) is then given by
\[
\frac{d\xi_T}{dn} = \frac{\partial \xi_T}{\partial a_{00}} \frac{da_{00}}{dn} + \frac{\partial \xi_T}{\partial a_{01}} \frac{da_{01}}{dn} + \frac{\partial \xi_T}{\partial a_{10}} \frac{da_{10}}{dn} + \frac{\partial \xi_T}{\partial a_{11}} \frac{da_{11}}{dn} \quad (17)
\]
and similarly for the other variables. Some of the right hand terms vanish, but most of them are always different from zero. Which terms vanish depends on the solved variable and the derivative which is being considered. To determine the error on a subsequent quantity like the tagging efficiency of the auxiliary tagger \( S \) (eq. 9) accurately, its dependences on previously solved-for quantities are substituted to obtain a function of the form

\[
\epsilon_S = \epsilon_S(a_{00}, a_{01}, a_{10}, a_{11}, b_{00}, b_{01}, b_{10}, b_{11}).
\]

The derivatives can then be determined as above to compute the final error in this quantity. This way of determining the errors has also the advantage that their magnitude does not depend on the order in which the unknowns have been solved.

4. Performance

The system of equations does not address charm flavour sample content. Other methods like fitting of muon in jets relative transverse momentum sample distributions to templates of different jet flavour contents \((b, c\) and light\) rely on simulation and the \(c\) and light flavour content templates are typically difficult to distinguish [9]. Within the system of eight equations the \(c\) flavour content is predominantly absorbed into the light flavour subsample. In this way the method is able to disentangle self-consistently the heavy and light flavour content of two given samples. However it is not possible to distinguish between light and \(c\) flavour contents. More details about this problem can be found in [2].

As a concrete example let’s consider two data samples \(n, p\) and their corresponding tagged subsamples

\[
\begin{align*}
n &= 758925, \\
n_T &= 73076, \\
n_S &= 376891, \\
n_{TS} &= 49810, \\
p &= 11082, \\
p_T &= 2406, \\
p_S &= 7198, \\
p_{TS} &= 1778.
\end{align*}
\]

(19)

The solution of the unknown quantities and their errors, determined as explained in the last section, are given by

\[
\begin{align*}
\epsilon_T &= 0.298 \pm 0.032, \\
f_T &= 0.026 \pm 0.005, \\
\epsilon_S &= 0.751 \pm 0.007,
\end{align*}
\]
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\[ f_S = 0.408 \pm 0.016, \]
\[ n_b = 195691 \pm 25645, \]
\[ n_q = 563234 \pm 24670, \]
\[ p_b = 7794 \pm 978, \]
\[ p_q = 3288 \pm 986. \]

This example shows typical numbers of a lifetime based tagger $T$ to be probed and an auxiliary de-correlated tagger $S$, needed to solve the system of equations. The denominators

\[ n_T - n f_T = 53344 \]
\[ n_T - n \epsilon_T = 73076 \]
\[ \epsilon_T - f_T = 0.272 \]

are far enough from singularities to ensure reasonably small errors on the solved quantities. If initial conditions have been chosen such that the solutions are getting close to a singularity, the computed errors diverge, indicating that an ill-posed problem is attempted to be solved. In this way one is protected against the misuse of poorly

\[ \begin{align*}
\Delta \epsilon_S / \epsilon_S & \equiv n = 758925 \\
n_T & \equiv 73076 \\
n_S & \equiv 376891 \\
p & \equiv 11082 \\
p_T & \equiv 2406 \\
p_S & \equiv 7198 \\
p_{TS} & \equiv 1778
\end{align*} \]

**Figure 1.** The relative error of the tagging rate $\epsilon_S$ as a function of the denominator $n_T - n f_T$, which is needed for the computation of $\epsilon_S$. The scan over the singularity has been achieved in varying the known quantity $n_{TS}$. Each dot corresponds to a solution of $n_{TS}$. The interpolation function has been obtained with cubic splines.
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adjusted working points of the taggers and badly chosen data samples. To minimize the errors it is convenient to use working points of the tagging algorithms which are far away from the singularities. In addition the heavy flavour content of the two data samples should not be too similar to each other, which would be the case if their heavy flavour contents would be consistent with each other within errors. In practice the two data samples can be realized by means of two different trigger requirements, one for each sample. An appropriate choice are jet only triggers on the one hand and muon plus jets triggers on the other hand. Since muons in jets indicate the presence of heavy flavour decays, the later category of triggers will provide a sample enhanced in heavy flavour content with respect to the former one.

To demonstrate the behaviour of initial conditions approaching a singularity the input values of the example given by eqs. 19 have been taken, with exception of the number of double tagged jets \( n_{TS} \) which has been varied. Fig. 1 shows the relative error \( \Delta \epsilon_S / \epsilon_S \) as a function of the denominator \( (n_T - n_{fT}) \) on which the tagging efficiency \( \epsilon_S \) depends. The values of the varied variable \( n_{TS} \) are also indicated. The relative error \( \Delta \epsilon_S / \epsilon_S \) exceeds unity while approaching the singularity. The relative error is monotonically decreasing from the singularity to the edges of the allowed phase space \( 0 < n_{TS} < \min(n_T, n_S) \). Pseudoexperiments have been conducted to verify that the computed efficiency \( \epsilon_S \) is also gaussian distributed in the vicinity of the singularity around two different central values \( n_{TS} = 35945 \) for which \( \Delta \epsilon_S / \epsilon_S \simeq 1 \) and \( n_{TS} = 36200 \) for which \( \Delta \epsilon_S / \epsilon_S \simeq 10 \). Furthermore the determined errors of the tagging efficiency and fake rate of the probed tagger have been checked for coverage by means of pseudoexperiments where the known quantities have been varied within their errors (see e.g. eqns. 15 for the errors of the sample \( n \) and corresponding subsamples).

Different working points of the taggers can be probed to maximize the denominators and minimize the errors on the most important quantities of interest, which are the efficiency and fake rate of the probed tagger. Their errors enter among others into the systematics of cross section measurements and limit calculations of searches for new physics where heavy flavour jets are involved.

5. Conclusions

An algebraic way of determining heavy and light flavour jet tagging efficiencies has been discussed. The analytical solution of a system of eight non-linear equations has been obtained by means of resultants. Its singularities suggest prescriptions to prevent badly chosen sample flavour compositions and working points of the used tagging algorithms. Errors are obtained by gaussian error propagation, taking correlations between the samples and subsamples into account. They diverge as one approaches the singularities making the method robust against its usage at badly chosen working points and allowing for optimisation.
Acknowledgements

Thanks to many colleagues of the DØ collaboration for useful discussions. This work has been supported by BMBF, DFG, a Marie Curie Early Stage Research Training Fellowship of the European Community’s Sixth Framework Programme under contract number MRTN-CT-2006-035606 and by the Commissariat à l’Energie Atomique and CNRS/Institut National de Physique Nucléaire et de Physique des Particules, France.

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