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Deterministic annealing as a jet clustering algorithm in hadronic collisions

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Abstract

We show that a general purpose clusterization algorithm, deterministic annealing, can be adapted to the problem of jet identification in particle production by high energy collisions. In particular, we consider the problem of jet searching in events generated at hadronic colliders. Deterministic annealing is able to reproduce the results obtained by traditional jet algorithms and to exhibit a higher degree of flexibility.

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1. Introduction

In high energy hadron–hadron collisions, events with high transverse energy are characterized by highly collimated particle jets, reflecting hard scattering processes at parton level. Radiation and pair production processes hide the information on the original partons momenta. To bridge the gulf between experimental results expressed in terms of hadron properties, and the theory, whose ingredients are quarks and gluons, a reconstruction processes is needed. By this process hadrons in the final states are grouped in jets and many dedicated algorithms have been proposed to this purpose. These algorithms, that shall be reviewed in Section 2, appear to be reasonable recipes taking into account geometrical considerations and theoretical prescriptions. It can be guessed that in this way one is solving an optimization problem, trying to minimize some cost functions. This is exactly at the basis of the so-called clustering problem. Here one looks for the optimal partition of a given set of objects in classes

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on the ground of some similarity property. This task is performed minimizing a prescribed cost function that is to be adapted to the problem under investigation. In a recent paper [1] it has been shown that a particular clustering algorithm, the so-called deterministic annealing (DA) [2–4], can be adapted to the study of the hadronic jets in high energy e^+e^- scattering. Essentially, DA can give the same results of the standard Durham algorithm in a faster way, as a consequence of a lower computational complexity. In this work we try to extend the use of DA to hadron–hadron collisions taking into account the peculiarities of the jet production in this type of interaction. In particular, in this kind of interactions only a part of the particles in the final state can be associated to partons coming from a hard scattering process. Deterministic annealing, in a version that allows data analysis in terms of a number of clusters either fixed or variable, will be presented in Section 3. In Section 4 results from the application of this method to simulated events will be presented and compared with those obtained by a Cone algorithm. Section 5 is dedicated to comments and conclusions.

2. Jet clustering algorithms

The need to associate energy and momentum of particles in the final state to the four-momentum of unobservable partons is realized through jet clustering algorithms.[1] The most common of them can be classified in two categories:

- Association algorithms that use an iterative procedure. For every pair of particles with four-momentum p_i and p_j, a test variable $y_{i,j} = f(p_i, p_j)$ is calculated. This test variable is then compared to a given threshold parameter y_{cut} and the pair is recombined into a new pseudo-particle k of four-momentum $p_k = p_i + p_j$ (E scheme, but other schemes have also been considered) provided that $y_{ij} \leqslant y_{\text{cut}}$. The algorithm is then reiterated to the new set of (pseudo) particles and it stops when, for all pairs, $y_{ij} \geqslant y_{\text{cut}}$. The number of pseudoparticles at the end of the algorithm counts the number of jets, which is therefore fixed by y_{cut}. This scheme has been implemented in various algorithms: JADE [7,8], Durham [9–11]), Cambridge [12].
- To a second class belong algorithms that associate particles in a jet only on the ground of geometrical properties. The prototype for them is the Cone algorithm defined in the Snowmass Convention [13]. Here in the first step the few particles having a transverse energy E_T greater than a fixed threshold E_T^0 are selected as *seeds* for jets. Subsequently the particles lying in a cone of given radius R_0 in the pseudorapidity-azimuth plane around each seed are associated with a jet, whose direction is fixed by an iterative procedure. More refined approaches consider the possibility of recombination and splitting of these proto-jets.

Here we stress an important difference between these two categories. While for the algorithms of the first kind jets include all the particles and their number can be fixed a priori, for the algorithms of the second kind the number of jets is essentially determined by the number of particles used as seed and a varying part of particles is excluded from the classification. This is the reason why the former scheme is used in the case of electron–positron scattering and the latter in the case of hadronic diffusions, where not all the particles are produced in hard interactions.

3. Deterministic annealing

Deterministic annealing is a general purpose clustering algorithm inspired by an analogy to the annealing procedure that consists of maintaining a system at thermal equilibrium while gradually lowering the temperature. The process assures that, in the limit of low temperature, the global free energy minimum is attained. The word *deterministic* refers to the fact that, as we shall see, thermal equilibrium is obtained minimizing directly the free energy, in opposition to the stochastic simulation used by simulated annealing [14]. We introduce here a formulation of DA called mass-constrained clustering (MCC) [3,4] that is particularly suitable for our application. In effect in this formulation the number of clusters is not fixed a priori, as it

[1] For a review of these and other jet algorithms see [5]. For a review of the Monte Carlo generators and their connections with the jet algorithms see [6].

happened in the precedent application of DA to the jet searching problem [1], but is the result of the calculation.

For each event we are analyzing we consider two sets, the set of the particle momenta that we denote $\mathbf{x}_k$ and the set of the momenta of the jets denoted $\mathbf{y}_i$. The MCC approach introduces an infinite number of tentative jets; at each stage of the annealing process only a limited portion of them are distinct, so one introduces the frequency p_i of jets with momentum $\mathbf{y}_i$. One defines also a distance $d(\mathbf{x}_k, \mathbf{y}_i)$ between each particle and each effective jet. The global distortion D is defined as

$$D = \sum_k \sum_i p(\mathbf{x}_k, \mathbf{y}_i) d(\mathbf{x}_k, \mathbf{y}_i) = \sum_k p(\mathbf{x}_k) \sum_i p(\mathbf{y}_i|\mathbf{x}_k) d(\mathbf{x}_k, \mathbf{y}_i), \quad (1)$$

where $p(\mathbf{x}_k, \mathbf{y}_i)$ is the joint probability distribution, $p(\mathbf{x}_k)$ is the probability of particle k and $p(\mathbf{y}_i|\mathbf{x}_k)$ is the conditional probability relating particle k with jet i, i.e., the probability to associate $\mathbf{x}_k$ with jet i. A possible choice for the momenta $\mathbf{x}_k$ and $\mathbf{y}_i$ is represented by (η, ϕ, E_T), where η is the pseudorapidity, ϕ the azimuth and E_T the transverse energy. In this case for the distance one can use the squared error distortion

$$d(\mathbf{x}_k, \mathbf{y}_i) = (\eta_k - \eta_i)^2 + (\phi_k - \phi_i)^2, \quad (2)$$

and, to give more emphasis to high E_T particles that have more information about the correct jet direction, the following definition for the particle weight $p(\mathbf{x}_k)$ in Eq. (1)

$$p(\mathbf{x}_k) = \frac{E_T^k}{\sum_k E_T^k}. \quad (3)$$

Following the analogy with a statistical physics system, D plays the role of the internal energy which, in the limit of zero temperature, one wants to minimize. In this limit one obtains the hard clustering solution, in which the association probabilities are zero or one. At finite temperature, instead, it is the minimum of the Helmholtz free energy F that determines the distribution at thermal equilibrium. This minimum is given by:

$$F^* = -T \sum_k \ln Z_k, \quad (4)$$

where Z_k is the partition function for the single particle

$$Z_k = \sum_i p_i e^{-d(\mathbf{x}_k, \mathbf{y}_i)/T}. \quad (5)$$

As a consequence the conditional probabilities are given by the Gibbs distribution

$$p(\mathbf{y}_i|\mathbf{x}_k) = \frac{p_i e^{-d(\mathbf{x}_k, \mathbf{y}_i)/T}}{Z_k}. \quad (6)$$

Imposing the free energy minimization under the constraint $\sum_i p_i = 1$, one obtains that the optimal set of jet vectors $\{y_i\}$ must satisfy the equations

$$\sum_k p(\mathbf{x}_k) p(\mathbf{y}_i|\mathbf{x}_k) \nabla_{\mathbf{y}_i} d(\mathbf{x}_k, \mathbf{y}_i) = 0, \quad (7)$$

while

$$p_i = \sum_k p(\mathbf{x}_k) p(\mathbf{y}_i|\mathbf{x}_k) = p(\mathbf{y}_i). \quad (8)$$

From Eq. (7) one obtains that the jet momenta are determined, for a squared error distortion $d(\mathbf{x}_k, \mathbf{y}_i) = |\mathbf{x}_k - \mathbf{y}_i|^2$, by

$$\mathbf{y}_i = \frac{\sum_k \mathbf{x}_k p(\mathbf{x}_k) p(\mathbf{y}_i|\mathbf{x}_k)}{p(\mathbf{y}_i)}. \quad (9)$$

The annealing process starts at high temperature. From (6) it is clear that the association probabilities are uniform, the system is completely disordered and the jet set collapses to a single point. This unique jet has $p(y_1) = 1$, every particle is associated with this jet with probability 1, $p(\mathbf{y}_1|\mathbf{x}_k) = 1$, and Eq. (9) gives the position of the centroid of the momenta set $\mathbf{y}_1 = \sum_k p(\mathbf{x}_k)\mathbf{x}_k$. During the cooling process one encounters phase transitions which consist of an increase in the number of effective jets through a sequence of jet splitting. The temperature plays the role of the resolution parameter at which the data set is clustered and a complete hierarchical clustering can be obtained up to the extreme situation at zero temperature when there is a jet for each particle. This process is described in Fig. 1 where the behavior of the free energy F as a function of $\beta = 1/T$ is shown for a typical event among those analyzed in the next section.

From a practical point of view, mass constrained clustering can be implemented by an algorithm that here we briefly sketch. Starting from a low value of β one introduces two jets with coordinates slightly

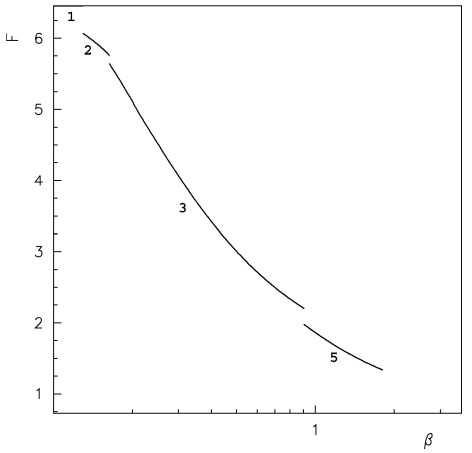

Fig. 1. The phase diagram for a simulated p–p scattering event (see Section 4).

perturbed with respect to the centroid coordinates and equal probability for every point to be associated with each cluster. Then one minimizes the free energy iterating the equations:

$$p(\mathbf{y}_i) = \sum_k p(\mathbf{x}_k)\, p(\mathbf{y}_i|\mathbf{x}_k), \tag{10}$$

$$p(\mathbf{y}_i|\mathbf{x}_k) = \frac{p(\mathbf{y}_i) e^{-\beta d(\mathbf{x}_k,\mathbf{y}_i)}}{\sum_j p(\mathbf{y}_j) e^{-\beta d(\mathbf{x}_k,\mathbf{y}_j)}}, \tag{11}$$

$$\mathbf{y}_i = \frac{\sum_k \mathbf{x}_k p(\mathbf{x}_k)\, p(\mathbf{y}_i|\mathbf{x}_k)}{p(\mathbf{y}_i)}, \tag{12}$$

until one finds convergence in $\mathbf{y}_i$. These equations correspond to the description given by Eqs. (5), (6), (8), (9). If β is low enough, it comes out that these two clusters are coincident. The next step is to cool the system, $\beta \to \alpha\beta$ $(\alpha > 1)$, always iterating equations (10)–(12) until a solution corresponding to two different jets (the first phase transition) is encountered. Subsequently one goes on by introducing, for each jet location, two perturbed jets which share the association probability of each particle, raising β and determining the new jets momenta. Each pair of jets will be merged until a critical β is reached, in which case one of the pairs will originate two effective jets. The process will be stopped when a sufficient resolution (β value or number of jets) is reached. We need to perturb the solution found at the $(n-1)$th step in β before using it as a starting point for the nth step. The reason is that it is still a fixed point for Eqs. (10)–(12) even if the phase transition has been crossed; however, it corresponds to a local minimum of the free energy, not to a global one.

In the next section we present our results compared with the Cone algorithm. For the time being we observe that the definitions (2), (3) have the interesting property that the coordinates of a jet, as defined by the Cone algorithm,

$$\eta^j = \frac{1}{E_T^j} \sum_{k\in j} E_T^k \eta^k, \qquad \phi^j = \frac{1}{E_T^j} \sum_{k\in j} E_T^k \phi^k,$$
$$E_T^j = \sum_{k\in j} E_T^k, \tag{13}$$

are exactly recovered by the DA algorithm in the limit of hard clustering ($\beta \to \infty$) with a fixed number of jets. In this limit, indeed, the association probabilities of each data point (particle) to a jet in Eq. (11) become 0 or 1 and from Eq. (12) one obtains exactly Eq. (13).

4. Results and discussions

We are now in position to explore the possibility of applying the mass constrained clustering version of deterministic annealing to the problem of jet search in hadronic colliders. To this purpose we generated 2000 events from proton–proton scattering at 14 TeV by the PYTHIA [15,16] Monte Carlo generator; a bias in the transverse energy E_T of the initial partons was introduced, corresponding to $E_T = 100$ GeV for 1000 events (sample A) and $E_T = 200$ GeV for the other 1000 events (sample B); initial and final state radiation was allowed. With this bias, a clear back-to-back two jet structure is expected. Results from application of DA where systematically compared with those obtained by the Cone algorithm described in Section 2: the Cone algorithm parameters, the transverse energy threshold E_T^0 and the cone radius R_0 have been fixed to 2 GeV and 0.7, respectively.

We calculated first two quantities that can be easily used for a comparison with the Cone algorithm. The first quantity is the mean distance of each particle from a jet j, defined as

$$\langle d \rangle = \frac{1}{N_c} \sum_{j=1}^{N_c} \frac{1}{p(\mathbf{y}_j)} \sum_k \sqrt{d(\mathbf{x}_k, \mathbf{y}_i)}\, p(\mathbf{x}_k)\, p(\mathbf{y}_i|\mathbf{x}_k), \tag{14}$$

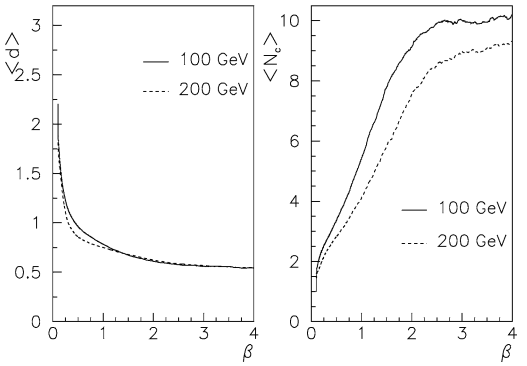

Fig. 2. First results from the application of DA algorithm to simulated events. Left side: $\langle d \rangle$, averaged over all the events, vs. β. Right side: the mean clusters number $\langle N_c \rangle$, vs. β.

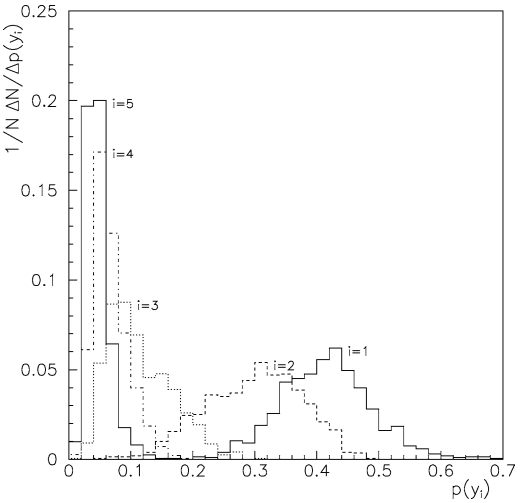

Fig. 3. The probability distributions for the five most probable clusters at $\beta = 1.4$.

where N_c is the number of clusters found. $\langle d \rangle$ is a decreasing function of β attaining its maximum value at $\beta = 0$, when there is only one cluster, and its minimum value, that is zero, at $\beta = \infty$ when every particle is a cluster by itself. This quantity, averaged over all the events, is shown, as a function of β in the left part of Fig. 2. We can see that there is no practical difference between the two analyzed samples: in either case $\langle d \rangle$ decreases quickly for low values of β, due to the growth in the number of clusters, then the descent becomes very slow. This behavior is the signal that the particle distribution in the events we are analyzing is such that the initial partition in few clusters is preserved when β is increased, apart from fragments of low weight. This robustness is confirmed by the second quantity we calculated, that is the mean number of clusters $\langle N_c \rangle$, whose behavior, as a function of β, is shown in the right part of Fig. 2. We see that the region of extreme fragmentation, that ends the clustering process, is far away at $\beta = 4$.

How to determine the two jet nature of our events? To answer this question we note that the DA recipe cannot be yet considered complete, because we still have two problems. The first problem is that the annealing process must be stopped at some β value to avoid the extreme cluster fragmentation produced by the $\beta \to \infty$ limit. The second problem arises because only part of the clusters can be attributed to the scattered partons. Therefore, once we choose β, we need also a criterion to select real jets from clusters. In the Cone algorithm these questions are controlled, as mentioned before, through two parameters: the transverse energy threshold E_T^0 and the cone radius R_0. The analogous role in DA algorithm is played by the parameter β and by a cut-off p_0 in the jet probability. We remember that DA introduces a probability measure for the clusters, the expression (10). A peculiarity of these probabilities is that the two jet nature of the events here analyzed produces, in the β region where $\langle d \rangle$ has a smooth behavior ($\beta \gtrsim 1$), two clusters of high probability, while to the remaining clusters only a small fraction of unity is assigned. To illustrate this feature the probability distributions for the five most probable clusters at $\beta = 1.4$ are shown in Fig. 3 for the events from sample A. A small value of cluster probability reflects the fact that the particles assigned to this cluster with a good association probability are few and have a small weight (transverse energy). So it is natural to consider jets only the clusters that survive a cut in the probability value. For example, we see in Fig. 4 how a threshold at $p_0 = 0.15$ influences the β dependence of the mean number of clusters N_c. Now this quantity goes rapidly to a value close to 2, i.e., the expected value for our sample.

At this point we are ready to illustrate how DA is able to reproduce the results obtained by the Cone algorithm. We performed the annealing process up to a β value of 1.4 and accepted only clusters with probability greater than $p_0 = 0.025$. With these values we obtained $\langle d \rangle = 0.69 \pm 0.11$, close to the value of $R_0 = 0.7$ used for the Cone algorithm. This could be

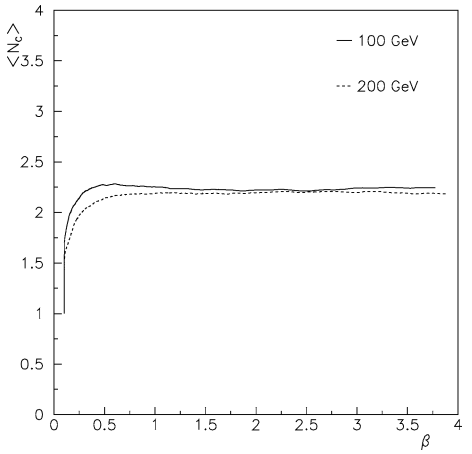

Fig. 4. The mean clusters number $\langle N_c \rangle$, vs. β. Only clusters having probability greater than $p_0 = 0.15$ have been considered.

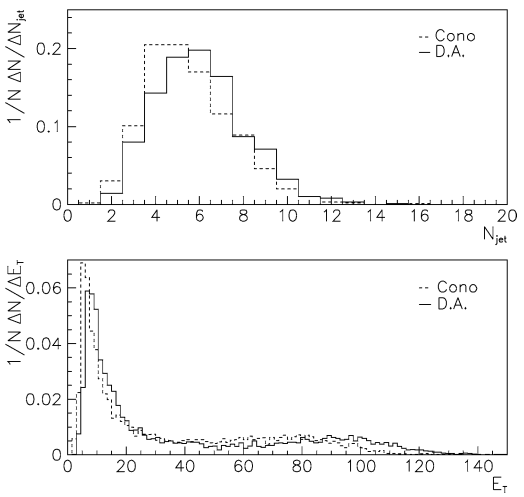

Fig. 5. The clusters number distribution (top) and the clusters transverse energy distribution (bottom) for the DA algorithm (solid line) and the Cone algorithm (dashed line). (Events are from sample A.)

expected because β has an effect on the association probability of a particle to a cluster (see (11)) that is comparable to that of the parameter R_0 for the Cone algorithm, if one puts $\beta \sim 1/2R_0^2$. No fine tuning of these parameters was performed, because this is not the aim of this Letter.

The comparison between the two algorithms is reported in Fig. 5 for two observables: the number of clusters and their transverse energy distribution. Some differences can be noted, in particular there is a more pronounced tail in the E_T distribution for the DA algorithm. This can be easily explained by the fact that, assuming $\langle d \rangle \sim R_0$, R_0 is a sharp threshold for the Cone algorithm, while for the DA algorithm $\langle d \rangle$ is the mean cluster radius. Another minor discrepancy is in the N_c-distribution that, for the DA algorithm, is slightly shifted to higher values of N_c. We could get rid of these differences modifying the values of β and p_0, but, as we said, we found this job useless, not least because we used a very simple Cone algorithm, where, for example, no recombination or splitting mechanism for proto-jets have been considered. A more interesting question to ask is which algorithm better reproduces the properties of the partons originating the jets. To this purpose we introduced two variables for each parton participating in the hard initial scattering and for the cluster nearest to it in direction. The first variable describes the ability to identify the parton direction:

$$\delta = \frac{1 - \cos\alpha}{2}, \tag{15}$$

where α is the angular separation between parton and jet axis. The other quantity measures the ability to trace the transverse energy of the parton:

$$\Delta = \frac{E_{T,p} - E_{T,c}}{E_{T,p}} \tag{16}$$

where $E_{T,p}$ and $E_{T,c}$ are the transverse energies of the parton and the jet, respectively. Their distributions for the two algorithms and the two data samples are shown in Fig. 6. We can see that, while for the δ distribution there are no practical differences between the two algorithms, DA seems to be more efficient in recovering the hard parton transverse energy.

5. Conclusions

We have compared the results found by the Cone algorithm with those obtained by a clustering algorithm based on the deterministic annealing procedure. The latter has been adapted to the process studied in this Letter, i.e., jet identification in particle production by high energy hadronic collisions, by introducing a suitable distortion measure and using temperature and cluster probability as parameters. Other choices are possible. For example, one could take into account that

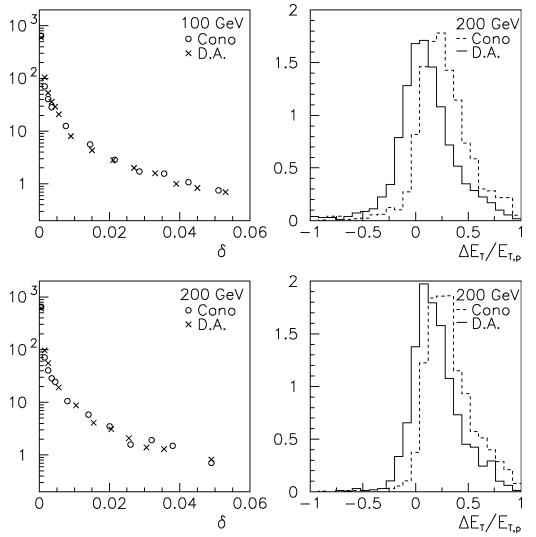

Fig. 6. The distribution of the angular distance between partons and jets (left) and the clusters transverse energy distribution (right) for the DA algorithm (solid line) and the Cone algorithm (dashed line).

the phase transition producing the splitting of a cluster occurs at a temperature proportional to the variance of the cluster itself [4]. So a characteristic of well defined clusters is that they are stable for a wide range of temperature and this stability property could be used in jet recognition.

From this preliminary analysis we cannot conclude that the DA algorithm should be preferred to the Cone algorithm, even if the good results for the number of clusters (4) and on the parton transverse energy should not be neglected. In any case we think that the jet-physics community should consider DA as a possible and serious alternative. The use of a geometrical definition of jet appear indeed too simplifying with respect to the theoretical descriptions. On the other hand, the DA algorithm looks at the properties of the density distribution in the momentum space, which is the reason why the recombination and splitting mechanisms are automatically incorporated.

Moreover, there is another general question that could be solved in this calculation scheme. It is true that the choice of jet definition is a matter of convention and that the important thing is to use the same definition in theoretical predictions and in experimental analysis. However, it cannot be considered satisfactory that, while there is a unique theory explaining jet production and properties, different definitions are used in hadronic and in leptonic collisions. The purpose of this Letter is to demonstrate that this difficulty could be overcome using the same algorithm, so that one can focus all the efforts in the most important question, i.e., the similarity property used to decide if two particles should be assigned to the same jet. Using a correct definition of this quantity, indeed, one can take into account important theoretical peculiarities, as infrared and collinear safety or formation of "ghost" and "junk" jets [17,18]. These kinds of similarity measure have been used, until now, only for e^+–e^- collisions and embodied in algorithms with poor performance, since they have to loop on all the particles' pairs. We hope to have clarified (see also [1]) that they could be used for any kind of interaction, without giving up the reduced computational complexity that geometrical algorithms share with the method we propose.

Acknowledgements

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