Fast NLO calculation of jet and charm production cross sections by pseudo-moment method

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Determination of the parton distribution functions requires repeated calculation of cross sections in the fitting procedure. In the standard method, limited computer time prevent us from using NLO calculation of QCD final state observables which involves time-consuming Monte Carlo integration. We describe a technique to circumvent the problem in Mellin-N space, in which NLO cross sections with arbitrary parton distributions are obtained quickly using the pre-calculated "pseudo moments" of partonic cross sections by a simple N-space integral.

1 Introduction

The Large Hadron Collider (LHC) explores unprecedentedly high energy regime. Discoveries and measurements at LHC are expected to clarify the mechanism of electroweak symmetry breaking and possibly unveil the underlying physics beyond the standard model. As the LHC is a QCD machine, how far these goals are achieved depends on our understanding of the QCD dynamics. Especially, precise knowledge of the parton distribution functions (PDFs) is fundamental for reducing the theoretical uncertainties in all the signal and background processes. Over the past years, major progress has been made in the determination of the PDFs, mainly owing to the precision DIS data from HERA. However, there are still relatively large uncertainties in, *e.g.*, the gluon distribution at large x and therefore continuous update of the PDF global analysis including the latest experimental data (and the future LHC data as well) is important.

One of the issues in the PDF global analysis is how to deal with the QCD final state observables. Since any NLO calculation of the QCD final state observables involves Monte Carlo integration with a large number of events, it is impractical to use it straightforwardly in the fitting procedure where the cross sections have to be calculated repeatedly with varying sets of the PDFs. A conventional way to avoid the problem is to apply the Kfactor approximation; the K-factor, $K = d\sigma^{\rm NLO}/d\sigma^{\rm LO}$, is calculated for a given set of PDFs and commonly used to calculate the NLO cross section for all the other sets of the PDFs. However, the K-factor actually depends on the PDFs and ignoring the dependence obscures the accuracy of the analysis. Therefore, it is desirable to introduce a more sophisticated way to calculate NLO cross sections such that the PDF dependence is separated from the phase space integration. There have been two ways proposed so far for that purpose. One is the "interpolation method" implemented in **fastNLO** [1] and **ApplGrid** [2], where the PDFs are interpolated and the phase space integration is performed with the PDFs replaced by the interpolation functions for each grid point in the x-space. Another is the "pseudo-moment method" formulated in the Mellin-N space [3, 4, 5], where the NLO cross section is given by a N-integral of the "pseudo moments" of the partonic cross section multiplied by the ordinary Mellin moments of the PDFs. In both methods, the phase space integration is performed independently from the PDFs and the result is stored as the pre-calculated data

with which the NLO cross section can be obtained for each set of the PDFs. In the present work, we apply the latter method^{*} which is convenient for combining with other programs in N-space. In the next section, we summarize the pseudo-moment method in detail.

2 Pseudo-moment method

The F_2 structure function measured in the inclusive DIS is expressed by a convolution

$$\frac{1}{x}F_2(x,Q^2) = \sum_k \alpha_s^k(\mu) \sum_a \int_x^1 \frac{dy}{y} C_{2,a}^{(k)}\left(\frac{x}{y},\frac{Q^2}{\mu^2}\right) f_a(y,\mu^2) , \qquad (1)$$

where $C_{2,a}$ and f_a are the coefficient function and parton distribution function for the *a*-th flavor, respectively. Hereafter, the renormalization and factorization scales are commonly taken to be μ for simplicity. Defining the Mellin moments of the PDFs as

$$f_a^N(\mu^2) \equiv \int_0^1 dx x^{N-1} f_a(x,\mu^2) , \qquad (2)$$

its inverse transform is given by

$$f_a(x,\mu^2) = \frac{1}{2\pi i} \int_{\mathcal{C}} dN x^{-N} f_a^N(\mu^2) , \qquad (3)$$

where the contour C in the complex-N plane is taken to be right to the rightmost singularity of $f_a^N(\mu^2)$. Substituting eq.(3) into eq.(1), we obtain the well-known expression

$$\frac{1}{x}F_2(x,Q^2) = \sum_k \alpha_s^k(\mu) \sum_a \frac{1}{2\pi i} \int_{\mathcal{C}} dN x^{-N} C_{2,a}^{(k),N} \left(\frac{Q^2}{\mu^2}\right) f_a^N(\mu^2) .$$
(4)

The convolution becomes a simple product in the Mellin-N space and the structure function is calculated by a Gaussian quadrature with $\mathcal{O}(100)$ evaluation points N_i on the integral contour. The coefficient functions at $N = N_i$ are calculated and stored in the initialization subroutine, and $f_a^{N_i}(\mu^2)$ is evaluated for each set of the initial PDFs generated in the fitting program.

Calculation of the QCD final state observables is more involved. Let us take, as an example, the inclusive jet cross section in hadronic process,

$$d\sigma = \sum_{k} \alpha_s(\mu)^k \sum_{a,b} \int dx_1 \int dx_2 d\hat{\sigma}^{(k)}_{ab \to jet+X}(x_1, x_2, \mu^2) f_a(x_1, \mu^2) f_b(x_2, \mu^2) , \qquad (5)$$

where $d\hat{\sigma}_{ab \to jet+X}^{(k)}$ is the partonic cross section calculated by Monte Carlo integration with experimental cuts. Since eq.(5) is not a simple convolution, it cannot be rewritten in the form of the inverse Mellin transform. Nonetheless, the PDFs and the partonic cross section can be separated in the N-space by substituting eq.(3) into eq.(5), as the following [3, 4, 5].

$$d\sigma = \sum_{k} \alpha_{s}(\mu)^{k} \sum_{a,b} \frac{1}{(2\pi i)^{2}} \int_{\mathcal{C}_{1}} dN_{1} \int_{\mathcal{C}_{2}} dN_{2} \left[d\hat{\sigma}_{ab}^{(k)} \right]_{N_{1},N_{2}} f_{a}^{N_{1}}(\mu^{2}) f_{b}^{N_{2}}(\mu^{2}) , \qquad (6)$$

^{*}It has already been used in the global analysis for the polarized PDFs by De Florian et al [6].

where the coefficients are defined by

$$\left[d\hat{\sigma}_{ab}^{(k)}\right]_{N_1,N_2} = \int dx_1 \int dx_2 d\hat{\sigma}_{ab\to \text{jet}+X}^{(k)}(x_1,x_2,\mu^2) x_1^{-N_1} x_2^{-N_2} .$$
(7)

Note that the coefficients are not same as the (double-) Mellin moments of the partonic cross section due to the experimental cuts, and therefore we call it "pseudo moments" instead. Parametrizing the integral contours as $N_{1,2} = c_0 + u_{1,2}e^{\pm i\phi}$ with $\pi/2 \leq \phi < \pi$, the above formula can be rewritten as

$$d\sigma = \sum_{k} \alpha_{s}(\mu)^{k} \sum_{a} \frac{1}{(2\pi i)^{2}} \int_{0}^{\infty} du_{1} \int_{0}^{\infty} du_{2}$$

$$\times \operatorname{Re} \left\{ e^{2i\phi} \left[d\hat{\sigma}_{a}^{(k)} \right]_{N_{1},N_{2}} H_{a}^{N_{1},N_{2}}(\mu^{2}) + \left[d\hat{\sigma}_{a}^{(k)} \right]_{N_{1},N_{2}^{*}} H_{a}^{N_{1},N_{2}^{*}}(\mu^{2}) \right\} ,$$

$$(8)$$

where $H_a^{N_1,N_2}$ is the double Mellin moment of the product of the PDFs for each partonic channel: $H_a(x_1, x_2; \mu^2) = \{f_g(x_1, \mu^2)f_g(x_2, \mu^2), \dots\}$. The pseudo moments (7) are nothing but the jet cross sections with the PDFs replaced by $x^{-N_{1,2}}$. Calculation of the pseudo moments has to be done for each experimental bin, but once it is done, the cross section for each set of the PDFs can be evaluated in a very short time. The pseudo-moment method is a general technique and can be applied to any observables such as the dijet cross section, heavy quark production, etc, which cannot be written in the form of the Melln convolution.

Now we compare numerically the cross sections calculated directly in x-space as in eq.(5) and those in N-space by the pseudo-moment method as in eq.(8). In both cases, the evolution program **QCD-PEGASUS** [7] was used with its default input PDFs (corresponding to the 2001/2 Les Houches benchmark tables [8]). Likewise, the integral contour for the N integration in the pseudo-moment method is taken to be same as the one for the inverse Mellin transform in **QCD-PEGASUS**: $N = c_0 + ue^{\pm i\phi}$ with $c_0 = 1.9$, $\phi = 3/4\pi$, and 144 evaluation points in the interval 0 < u < 80.

Figure 1 shows the relative error between those results for the inclusive jet production cross section in ep collision at HERA. Each bin corresponds to a set of (Q^2, E_T) and each group of 4 bins (corresponding to $E_T = 7, 11, 30, 50 \text{GeV}$ from left to right) corresponds to the same Q^2 bin (= 150 \text{GeV}^2 - 15000 \text{GeV}^2 from left to right). We see that the error is less than 0.01% over the whole range of the kinematics.

Figure 2 is same as Fig.1, but for the inclusive jet production at LHC. The left and right panel are for the central (0 < y < 0.8) and forward (2.5 < y < 3.2) rapidity



Figure 1: Comparison of N-space calculation and x-space calculation for the inclusive jet production in ep collision at HERA.

region, respectively. In both regions, the error is less than 0.01% except for the highest P_t bins, where the cross section is highly suppressed and the statistical errors are supposed to be large. Hence we confirm that calculation of the inclusive jet cross section in the pseudo-moment method has enough accuracy when the N-integral contour is commonly taken with the one for calculation of the PDFs and structure functions.



Figure 2: Same as Fig.1 but for the inclusive jet production in pp collision at LHC in the central rapidity region: y = 0 - 0.8 (left panel) and forward rapidity region: y = 2.5 - 3.2 (right panel).

3 Charm structure function

Another observable which plays an important role in the determination of the PDFs is charm structure function $F_2^{c\bar{c}}(x, Q^2, m^2)$. Factorization formula for $F_2^{c\bar{c}}$ up to NLO is given by

$$F_{2}^{c\bar{c}}(x,Q^{2},m^{2}) = \frac{Q^{2}\alpha_{s}(\mu)}{4\pi^{2}m^{2}} \int_{x}^{z_{\text{max}}} \frac{dz}{z} \left[e_{c}^{2}f_{g}\left(\frac{x}{z},\mu^{2}\right) c_{2,g}^{(0)} \right] \\ + \frac{Q^{2}\alpha_{s}^{2}(\mu)}{\pi m^{2}} \int_{x}^{z_{\text{max}}} \frac{dz}{z} \left[e_{c}^{2}f_{g}\left(\frac{x}{z},\mu^{2}\right) \left(c_{2,g}^{(1)} + \bar{c}_{2,g}^{(1)} \ln \frac{\mu^{2}}{m^{2}} \right) \\ + \sum_{i=q,\bar{q}} \left[e_{c}^{2}f_{i}\left(\frac{x}{z},\mu^{2}\right) \left(c_{2,i}^{(1)} + \bar{c}_{2,i}^{(1)} \ln \frac{\mu^{2}}{m^{2}} \right) + e_{i}^{2}f_{i}\left(\frac{x}{z},\mu^{2}\right) \left(d_{2,i}^{(1)} + \bar{d}_{2,i}^{(1)} \ln \frac{\mu^{2}}{m^{2}} \right) \right] \right],$$

$$(9)$$

where $e_c(e_i)$ is the charge of the charm (light) quark and m denotes the charm quark mass. The coefficient functions $c_{2,j}^{(0,1)}$, $\bar{c}_{2,j}^{(1)}$ and $d_{2,j}^{(1)}$, $\bar{d}_{2,j}^{(1)}$ are functions of $\eta = \frac{\hat{s}}{4m^2} - 1$ and $\xi = \frac{Q^2}{m^2}$ where \hat{s} is the partonic CM energy. They cannot be written in analytic functions except the dominant parts in the threshold and asymptotic regions. The remaining part was tabulated numerically by Riemersma et al. [9]. However, in order to calculate the charm structure function in the Mellin-space programs, N-space expressions of the coefficient functions are necessary. For that purpose, Alekhin and Blümlein [10] performed a polynomial fitting with the MINIMAX-method,

$$c_{2,g}^{(1)}(z,\xi)(\rho-z)^{\kappa} = \sum_{k=0}^{K} a_k(\rho) z^k , \qquad (10)$$

where $\rho = \frac{\xi}{\xi+4}$. The Mellin transform of this expression is given in terms of the beta function,

$$M[c_{2,g}^{(1)}(z,\xi)](N) = \sum_{k=0}^{K} a_k(\rho) \rho^{N+k-\kappa} B(N+k,1-\kappa) .$$
(11)

The coefficients $a_k(\rho)$ are interpolated in ρ space using the tabulated data. In the fitting procedure, these coefficient functions have to be calculated for each Q^2 value of the experimental bin, but are treated in the same way as the massless coefficient functions otherwise.

Figure 3 compares the x-space calculation using eq.(9) with the parametrization by Riemersma et al. and the N-space calculation using the inverse Mellin transform eq.(4) with the N-space expression in eq.(11). The comparison is made for each component of $F_2^{c\bar{c}}(x,Q^2,m^2)$: the LO, NLO gluon and NLO quark component, corresponding to the first, second and third line in eq.(9), respectively. We have taken $Q^2 =$ 30GeV^2 , $\mu^2 = Q^2 + m^2$ and the PDFs corresponding to 2001/2 Les Houches benchmark tables [8]). The figure demonstrates a good agreement between the results by these two calculation methods. We note that the relative error for the sum of all components is less than 0.1% in the entire range of x.



Figure 3: Comparison of N-space calculation and x-space calculation for components of the charm structure function $F^{c\bar{c}}(x, Q^2, m^2)$ at $Q^2 = 30 \text{GeV}^2$.

4 Summery

The pseudo-moment method enables us to perform fast NLO calculation of QCD final state observables with varying parton distributions which is required in the PDF global analysis. We demonstrated a good numerical agreement between the N-space calculation and the x-space calculation for the inclusive jet cross sections and charm structure function. The techniques described here will be implemented in our PDF global analysis in the future.

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