Extracting Parton Densities from Collider Data

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Abstract
Collider data can play an important role in determining the parton distribution functions of the nucleon. I present a formalism which makes it possible to use next-to-leading order calculations in such a determination, while minimizing the amount of numerical computation required.

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1. Introduction

Perturbative quantum chromodynamics gives an excellent description of short-distance scattering processes at present-day colliders. The perturbative description relies on our ability to compute short-distance matrix elements in nonabelian gauge theories. It also relies on our understanding of factorization, which permits a separation of the process-dependent short-distance aspects from the universal, process-independent long-distance ones. The long-distance parts of scattering processes are captured in the parton distribution functions of the scattering nucleon(s). Along with the running coupling $\alpha_s$, they are the only ingredients needed from outside perturbation theory for a description (up to subleading power corrections) of collider scattering processes. Precise knowledge of parton distributions is important in the quest for physics beyond the standard model. At current or planned high-energy colliders new physics must necessarily be detected against an omnipresent background of QCD or QCD-corrected events.

The momentum evolution of parton distribution functions and of the running coupling is also governed by perturbative equations, so that it is only their values at a fixed scale which are required inputs from outside perturbation theory. Such input parton distributions may someday be calculated on the lattice or by other nonperturbative means, but at present they must be extracted from experiments. The modern approaches [1,2] involve global fits of next-to-leading order theory to all available experiments. The experiments involve different scale arguments to the distribution functions, but as these are related by the above-mentioned perturbative evolution equation, we can regard the fits as determining the distributions at a certain fixed scale $Q_0$.

To date, it is primarily deeply-inelastic scattering data that has been used in the global fits. (There is some ad-hoc use of collider data; for example, MRS [1] make use of certain points from the lepton asymmetry distribution from CDF and D0, relying on the fact that NLO corrections are small for these points, and on the availability of an analytic calculation for this quantity.) Yet there is a wealth of collider data which may yield important constraints on the parton densities, in particular the gluon distribution. The latter enters into DIS calculations only at higher order in the coupling, but is a dominant contribution in hadron-hadron collisions.

The deeply-inelastic structure functions used in the fits can be described by a convolution of an analytically-known function with the parton distributions. This makes their use in a fit computationally feasible. In contrast, for next-to-leading order differential cross sections at colliders (both hadron-hadron and lepton-hadron), even the short-distance part must necessarily be calculated numerically. This is a consequence of the relatively complicated structure of phase space, once one allows for arbitrary experimental cuts and jet algorithm.

In principle, existing NLO jet programs can be used in the global fits. Were we to try to use
them, however, we would have to regenerate the parton distributions (for example, in the form of numerical tables) at each iteration of a fit, and then re-run the jet program given the new values. This latter part of this procedure would be extremely time-consuming, and completely impractical for fits requiring more than a handful of iterations.

Yet much of the calculation of a jet differential cross section — the jet algorithm and experimental cuts, the numerical integration over real emission, the balancing of real and virtual contributions — is in fact independent of the precise form of the parton distribution functions. Thus it would be useful to re-organize the calculation so as to minimize the amount of computational work needed at each iteration of a fit to experimental data.

One might imagine pre-generating values for a grid of parameter values, and interpolating between them to find the best fit, but if in a realistic case one has 15 parameters, and wants (say) to consider ranges discretized into 10 values each, one would have to generate $10^{15}$ different points, clearly a hopeless task.

Fortunately, there is a better way; read on to discover it. Graudenz et al. [3] have previously presented an approach to using certain jet distributions from lepton-proton scattering. The approach presented here has certain elements in common with theirs (such as the use of Mellin transforms), but is fully general. It can be applied to arbitrary differential distributions in both lepton-hadron and hadron-hadron scattering. It is also free of certain theoretical restrictions and numerical limitations present in their approach.

### 2. A Prototype

Let us first consider leading-order calculations for a glueball $G$ in a quarkless version of QCD. This will serve as a warm-up exercise for the real-world case.

In this case we have only one distribution to consider, $f_{g\to G}(x, Q^2)$. The total $n$-jet cross section, subject to experimental cuts, in glueball-glueball scattering, is given by

$$
\sigma_n = \int_0^1 \int_0^1 dx_1 dx_2 \int d\text{LIPS}(x_1 k_G + x_2 k'_G \to \{k_i\}_{i=1}^n) \\
\times f_{g\to G}(x_1, \mu^2_F(\{k_i\}, x_{1.2})) f_{g\to G}(x_2, \mu^2_F(\{k_i\}, x_{1.2})) \\
\times \alpha_s^n(\mu^2_R(\{k_i\}, x_{1.2})) \hat{\sigma}(gg \to \{k_i\}) J_{n\to n}(\{k_i\}),
$$

where LIPS stands for the Lorentz-invariant phase-space measure. In this equation, $\hat{\sigma}$ stands for the usual leading-order partonic differential cross section with the running coupling $\alpha_s$ set to 1, and $f_{g\to G}(x, \mu^2)$ is the gluon distribution inside the glueball. Note that the $k_i$ are implicitly dependent
on \( x_1 \) and \( x_2 \) as well. The renormalization and factorization scales \( \mu_R \) and \( \mu_F \) — typically something like a jet \( E_T \) — also depend on \( x_{1,2} \) and the final-state momenta (thereby violating, for example, one of the theoretical restrictions in the work of Graudenz et al. [3]).

The jet algorithm is represented by \( J_{n\to n} \), which evaluates to 1 if the original \( n \)-parton configuration yields \( n \) jets satisfying the experimental cuts, and 0 otherwise. The precise form of the jet algorithm is not important for the formalism presented here.

The parton distribution functions satisfy evolution equations, whose solutions can be written using a *universal* evolution operator \( E(x, \alpha_s(Q^2), \alpha_0) \). (The initial coupling \( \alpha_0 = \alpha_s(Q^2_0) \) is one of the parameters we will want to fit.) Explicit forms for the evolution operator can be found in the paper of Furmanski and Petronzio [4] and elsewhere. The solutions can be written in the form

\[
f_{g\to G}(x, Q^2) = E(x, \alpha_s(Q^2), \alpha_0) \otimes f_{g\to G}(x, Q^2_0),
\]

where

\[
A(x) \otimes B(x) = [A \otimes B](x) \equiv \int_0^1 dy \int_0^1 dz \, \delta(x - yz)A(y)B(z)
\]

defines the convolution symbol \( \otimes \).

A Mellin transformation turns these convolutions into multiplications,

\[
f^{z}_{g\to G}(Q^2) = E^z(\alpha_s(Q^2), \alpha_0) f^{z}_{g\to G}(Q^2_0),
\]

in which

\[
A^z = \int_0^1 dx \, x^{z-1} A(x)
\]

is the Mellin transform of \( A \).

To recreate the original function, use the inverse Mellin transform,

\[
A(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dz \, x^{-z} A^z.
\]

The contour should be chosen to the right of all the singularities of \( A^z \).

We can thus write

\[
f_{g\to G}(x, Q^2) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dz \, x^{-z} E^z(\alpha_s(Q^2), \alpha_0) f^{z}_{g\to G}(Q^2_0).
\]

All the parameters (except \( \alpha_0 \)) that we wish to fit are contained in \( f^{z}_{g\to G}(Q^2_0) \). This latter function is *independent* of all integration variables except \( z \), and thus can be pulled out of the numerical integrations in eqn. (2.1). The remaining \( z_{1,2} \) contour integrals are to be performed during the fitting procedure, but this involves only a double sum of the gluon distribution function multiplied by precomputed numerical coefficients. We will be able to make use of techniques described in
ref. [5] to find numerically efficient contours for the $z_i$ integrations. I postpone the discussion of the choice of contours, and the method for performing the contour integrals, to a later section.

Thus at each step of the fitting procedure, we must compute only

$$-rac{1}{4\pi^2} \int_{c-i\infty}^{c+i\infty} dz_1 \int_{c-i\infty}^{c+i\infty} dz_2 \, f_{g^-G}(Q_0^2) f_{g^-G}(Q_0^2) \Sigma_{z_1, z_2}^{z_1, z_2},$$

(2.8)

where $\Sigma_{z_1, z_2}$ are precomputed coefficients given by

$$\Sigma_{z_1, z_2} = \int_0^1 dx_1 dx_2 \int dLIPS(x_1 k_G + x_2 k_G' \to \{k_i\}_{i=1}^n)$$

$$\times x_1^{-z_1} x_2^{-z_2} E^{z_1}(\alpha_s(\mu_F^2(\{k_i\}, x_{1,2}), \alpha_0)) E^{z_2}(\alpha_s(\mu_F^2(\{k_i\}, x_{1,2}), \alpha_0))$$

$$\times \alpha_s^n(\mu_R^2(\{k_i\}, x_{1,2})) \delta(gg \to \{k_i\}) J_{n-n}(\{k_i\}).$$

(2.9)

Since $\Sigma$ contains all of the short-distance process-specific dynamics, but is independent of the parton distributions (and indeed, of the nature of the parent hadron), it is appropriate to call it a universal cross section, in this case to leading order in quarkless QCD.

This procedure works for the parameters in $f_{g^-G}(Q_0^2)$ because $\Sigma$ is independent of them. It does not work for $\alpha_0$, the remaining fit parameter, because cross sections and distributions depend on $\alpha_0$ in a (complicated) non-polynomial fashion. There are several approaches we can take here. The simplest is to generate the coefficients $\Sigma_{z_1, z_2}$ for a set of $\alpha_0$ around a “canonical” value (e.g. $\alpha_s(M_Z^2) = 0.117$), and then fit using interpolation. While this approach would be vastly too time-consuming for a large number of parameters, it is acceptable for a lone parameter.

In general, we don’t want to fit total cross sections, but rather differential distributions. The above discussions go through just as well for the latter.

3. Leading-Order Fits

Let us turn next to leading-order fits in the real world, specializing to the Tevatron. The formulæ are quite similar to those in the previous section, except that we must sprinkle a variety of indices in appropriate places.

The $n$-jet differential cross section (in the variable $X$) is now given by

$$\frac{d\sigma_{n \to n}^{LO}}{dX} = \sum_{ab} \int_0^1 dx_1 dx_2 \int dLIPS(x_1 k_p + x_2 k_p' \to \{k_i\}_{i=1}^n)$$

$$\times f_{a\to p}(x_1, \mu_F^2(\{k_i\}, x_{1,2})) f_{b\to p}(x_2, \mu_F^2(\{k_i\}, x_{1,2})) \delta(X - X(\{k_i\}))$$

$$\times \alpha_s^n(\mu_R^2(\{k_i\}, x_{1,2})) \delta^{LO}(ab \to \{k_i\}) J_{n-n}(\{k_i\}).$$

(3.1)
The partonic cross section \( \hat{\sigma} \) is implicitly summed over all different possible final states, and the partonic types \( a, b \) are summed over the gluon and all relevant quark and antiquark distributions.

Eqn. (2.4) is replaced by

\[
f_z^{a\rightarrow p}(Q^2) = E_{ab}^z(\alpha_s(Q^2), \alpha_0) f_z^{b\rightarrow \bar{p}}(Q_0^2).
\]

The matrix \( E^z \) is most easily expressed in a basis of the evolution eigendistributions \( q^-, q^+, q \), along with gluon distribution \( g \) and the quark singlet distribution \( S \). The initial parton distributions are often expressed in this basis as well, but we need the evolved distributions in the usual flavor basis. It is therefore convenient to use \( E^z \) in a form where its left index is in the flavor basis, and its right index is in the eigendistribution basis.

Each step of the fitting procedure involves the computation of

\[
-\frac{1}{4\pi^2} \int_{c-i\infty}^{c+i\infty} dz_1 \int_{c-i\infty}^{c+i\infty} dz_2 \ f_z^{a\rightarrow p}(Q_0^2) f_z^{b\rightarrow \bar{p}}(Q_0^2) \frac{d\Sigma_{a\rightarrow b}}{dX}
\]

(with implicit summation over \( a, b \)), where

\[
d\Sigma_{a\rightarrow b} = \int_0^1 \int_0^1 dx_1 dx_2 \int d\text{LIPS}(x_1 k_p + x_2 k_{\bar{p}} \rightarrow \{k_i\}_{i=1}^n) \\
\times x_1^{z_1} x_2^{z_2} E_{a'a}(\alpha_s(\mu_F^2(\{k_i\}, x_{1,2})), \alpha_0) E_{b'b}(\alpha_s(\mu_F^2(\{k_i\}, x_{1,2})), \alpha_0) \\
\times \alpha_n^2(\mu_R^2(\{k_i\}, x_{1,2})) \sigma^{LO}(a'b' \rightarrow \{k_i\}) J_{n\rightarrow n}(\{k_i\}) \delta(X - X(\{k_i\})).
\]

In a numerical computation, the delta function is implemented by binning in \( X \).

### 4. Next-to-Leading Order Fits

At next-to-leading order, the structure of the cross section is more complicated; we must combine virtual corrections with real-emission ones. This is a delicate procedure, because each of these contributions is independently infrared divergent, and only their sum is well-defined. Moreover, from a practical point of view, the only practical infrared regulator is dimensional regularization, which does not mesh naturally with numerical calculations. The notion of a parton resolution — most simply an invariant mass \( s_{\text{min}} \), with a pair of partons \( (i, j) \) unresolvable if \( (k_i + k_j)^2 < s_{\text{min}} \) — offers a safe passage through these treacherous divergences and cancellations. The basic idea is to evaluate analytically the infrared-divergent contributions from real emission over the phase space for (color-adjacent) unresolved partons, and to add this contribution to the virtual corrections. The poles in the dimensional regulator \( \epsilon \) then vanish, and one can take the four-dimensional limit of all expressions. The remaining contributions, over the phase-space for resolved partons,
are computed numerically. Upon adding the two contributions, the dependence on the resolution parameter disappears (in the limit $s_{\text{min}} \to 0$) and one obtains the next-to-leading order differential cross section. Color ordering plays an important role because the notion of resolved or unresolved partons is defined independently for each color permutation.

Several variants of this approach to general processes in collider physics have been presented in the literature, in particular the ‘slicing’ [6,7] and ‘subtraction’ [8,9] ones. The details are again not important for our purposes. The exposition below assumes the use of either the pure slicing or a ‘restricted subtraction’ method, for which a subtraction of singular pieces is performed only inside the region $s_{\text{sing}} < s_{\text{min}}$. Analogous formulæ can however be written down for the subtraction method of refs. [8,9]. I shall indicate the restriction to resolved configurations via an additional superscript $R$ on, and an additional argument $s_{\text{min}}$ to, the appropriate leading-order partonic cross-section. Similarly, a superscript $U$ will denote the restriction to unresolved configurations.

Thus

$$\frac{d\delta\sigma_{\text{NLO}}}{dX} = \frac{d\sigma_{\text{LO}}}{dX} + \frac{d\delta\sigma_{\text{NLO},\text{U}}}{dX} + \frac{d\delta\sigma_{\text{NLO},\text{R}}}{dX}. \quad (4.1)$$

The contribution of configurations with $n + 1$ resolved partons is,

$$\frac{d\delta\sigma_{\text{NLO},\text{R}}}{dX} = \sum_{ab} \int_{0}^{1} \int_{0}^{1} dx_1 dx_2 \int \text{dLI}(x_1 p + x_2 \bar{p} \to \{k_i\}_{j=1}^{n+1})$$

$$\times f_{a\to p}(x_1, \mu^2 f_1(\{k_i\}, x_1, x_2)) f_{b\to \bar{p}}(x_2, \mu^2 f_1(\{k_i\}, x_1, x_2)) \delta(X - X(\{k_1\}))$$

$$\times \alpha_s^{n+1}(\mu_s^2(\{k_i\}, x_1, x_2)) \frac{\sigma_{\text{LO},\text{R}}}{dX}(ab \to \{k_i\}; s_{\text{min}}) J_{n\to n+1}(\{k_i\}). \quad (4.2)$$

In this equation, $J_{n\to n+1}(\{k_i\})$ evaluates to one if a given $(n + 1)$-parton configuration yields $n$ detected jets, and vanishes otherwise. It is crucial that both the jet algorithm and the differential cross section under consideration be infrared-safe, to wit the treatment of an event must not change under the addition of an arbitrarily soft gluon, or the splitting of any parton into two collinear partons. Otherwise, the details of the jet algorithm are again unimportant for the formalism presented here.

What is more important for us is the structure of the unresolved pieces,

$$\frac{d\delta\sigma_{\text{NLO},\text{U}}}{dX} = \frac{d\delta\sigma_{\text{NLO},\text{F}}}{dX} + \frac{d\delta\sigma_{\text{NLO},\text{C}}}{dX}. \quad (4.3)$$

The first term combines the virtual corrections with the singular integrals over the unresolved phase space, in a crossing-invariant fashion. This term would be present whether or not the initial
state contained colored partons,

\[
\frac{d\delta\sigma_{n}^{NLO}}{dX} = \sum_{ab} \int_{0}^{1} dx_{1} dx_{2} \int d\text{LIPS}(x_{1}k_{p} + x_{2}k_{p} \rightarrow \{k_{i}\}_{i=1}^{n})
\times f_{a\rightarrow p}(x_{1}, \mu_{F}^{2}(\{k_{i}\}, x_{1,2})) f_{b\rightarrow p}(x_{2}, \mu_{F}^{2}(\{k_{i}\}, x_{1,2})) \delta(X - X(\{k_{i}\}))
\times \alpha_{s}^{n+1}(\mu_{R}^{2}(\{k_{i}\}, x_{1,2})) \hat{\delta}\sigma_{NLO}^{ab \rightarrow \{k_{i}\} ; s_{\text{min}}} J_{n \leftarrow n}(\{k_{i}\}).
\]  

(4.4)

The second term crosses colored partons from the final state to the initial state; it is thus absent in e^+ e^- scattering. In our case, it takes the form

\[
\frac{d\sigma_{n}^{NLO,C}}{dX} = \sum_{ab} \int_{0}^{1} dx_{1} dx_{2} \int d\text{LIPS}(x_{1}k_{p} + x_{2}k_{p} \rightarrow \{k_{i}\}_{i=1}^{n})
\times \left[C_{a\rightarrow p}(x_{1}, \mu_{F}^{2}(\{k_{i}\}, x_{1,2}); s_{\text{min}}) f_{b\rightarrow p}(x_{2}, \mu_{F}^{2}(\{k_{i}\}, x_{1,2}))
+ f_{a\rightarrow p}(x_{1}, \mu_{F}^{2}(\{k_{i}\}, x_{1,2})) C_{b\rightarrow p}(x_{2}, \mu_{F}^{2}(\{k_{i}\}, x_{1,2}); s_{\text{min}}) \right] \delta(X - X(\{k_{i}\}))
\times \alpha_{s}^{n+1}(\mu_{R}^{2}(\{k_{i}\}, x_{1,2})) \hat{\sigma}_{\text{LO}}^{ab \rightarrow \{k_{i}\} ; s_{\text{min}}} J_{n \leftarrow n}(\{k_{i}\}),
\]  

(4.5)

where \(C_{a\rightarrow p}\) is a crossing function as introduced in ref. [7]. The crossing functions are factorization-scheme dependent; they can be expressed in terms of scheme-independent functions \(A_{a\rightarrow p}\) and scheme-dependent functions \(B_{a\rightarrow p}\) as follows,

\[
C_{a\rightarrow p}(x, Q^{2}) = \left(\frac{N}{2\pi}\right) \left[A_{a\rightarrow p}(x, Q^{2}) \ln \left(\frac{s_{\text{min}}}{Q^{2}}\right) + B_{a\rightarrow p}(x, Q^{2})\right],
\]  

(4.6)

with

\[
A_{a\rightarrow p}(x, Q^{2}) = K_{a\rightarrow b}^{A}(x) \otimes f_{b\rightarrow p}(x, Q^{2}),
B_{a\rightarrow p}(x, Q^{2}) = K_{a\rightarrow b}^{B}(x) \otimes f_{b\rightarrow p}(x, Q^{2}).
\]  

(4.7)

Expressions for the kernels \(K^{A,B}\) are given in ref. [7], and expressions for their Mellin moments \(K^{A,z}\) and \(K^{B,z}\) in ref. [5].

With these moments, we can define

\[
K_{a\rightarrow b}^{C,z} = \left(\frac{N}{2\pi}\right) \left[K_{a\rightarrow b}^{A,z} \ln \left(\frac{s_{\text{min}}}{Q^{2}}\right) + K_{a\rightarrow b}^{B,z}\right];
\]  

(4.8)

this allows us to write

\[
C_{a\rightarrow p}^{z}(Q^{2}) = K_{a\rightarrow b}^{C,z} f_{b\rightarrow p}^{z}(Q^{2}),
\]  

(4.9)

and then using eqn. (3.2),

\[
C_{a\rightarrow p}^{z}(Q^{2}) = K_{a\rightarrow b}^{C,z} E_{bc}^{z}(\alpha_{s}(Q^{2}), \alpha_{0}) f_{c\rightarrow p}^{z}(Q_{0}^{2}).
\]  

(4.10)
Each step of the fitting procedure involves the computation of the same quantity as in eqn. (3.3), where now

$$\frac{d\Sigma^{z_1,z_2}}{dX} = \frac{d\Sigma^{LO;z_1,z_2}}{dX} + \frac{d\delta\Sigma^{NLO,U;z_1,z_2}}{dX} + \frac{d\delta\Sigma^{NLO,R;z_1,z_2}}{dX}$$

$$= \frac{d\Sigma^{LO;z_1,z_2}}{dX} + \frac{d\delta\Sigma^{NLO,F;z_1,z_2}}{dX} + \frac{d\delta\Sigma^{NLO,C;z_1,z_2}}{dX} + \frac{d\delta\Sigma^{NLO,R;z_1,z_2}}{dX}.$$  \hspace{1cm} (4.11)

The first term, \(d\Sigma^{LO;z_1,z_2}/dX\), is given by eqn. (3.4); the latter quantities are given by the following equations,

$$\frac{d\delta\Sigma^{NLO,R;z_1,z_2}}{dX} = \int_0^1 \int_0^1 dx_1 dx_2 \int d\text{LIPS}(x_1 k_p + x_2 k_p \to \{k_i\}_{i=1}^{n+1}) \delta(X - X(\{k_i\}))$$

$$\times x_1^{-z_1} x_2^{-z_2} E_{a'a}^{z_1}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0) E_{b'b}^{z_2}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0)$$

$$\times \alpha_s^{n+1}(\mu_R^2(\{k_i\}, x_1, 2)) \delta^{LO}(a'b' \to \{k_i\}; s_{\text{min}}) J_{n\to n+1}(\{k_i\}).$$  \hspace{1cm} (4.12)

$$\frac{d\delta\Sigma^{NLO,F;z_1,z_2}}{dX} = \int_0^1 \int_0^1 dx_1 dx_2 \int d\text{LIPS}(x_1 k_p + x_2 k_p \to \{k_i\}_{i=1}^{n+1}) \delta(X - X(\{k_i\}))$$

$$\times x_1^{-z_1} x_2^{-z_2} E_{a'a}^{z_1}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0) E_{b'b}^{z_2}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0)$$

$$\times \alpha_s^{n+1}(\mu_R^2(\{k_i\}, x_1, 2)) \delta^{NLO}(a'b' \to \{k_i\}; s_{\text{min}}) J_{n\to n}(\{k_i\}).$$  \hspace{1cm} (4.13)

$$\frac{d\delta\Sigma^{NLO,C;z_1,z_2}}{dX} = \int_0^1 \int_0^1 dx_1 dx_2 \int d\text{LIPS}(x_1 k_p + x_2 k_p \to \{k_i\}_{i=1}^{n+1}) \delta(X - X(\{k_i\}))$$

$$\times x_1^{-z_1} x_2^{-z_2} \left[ K^{C;z_1}_{a'\leftarrow a} E_{a'a}^{z_1}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0) E_{b'b}^{z_2}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0)$$

$$+ E_{a'a}^{z_1}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0) K^{C;z_2}_{b'\leftarrow b} E_{b'b}^{z_2}(\alpha_s(\mu_F^2(\{k_i\}, x_1, 2)), \alpha_0) \right]$$

$$\times \alpha_s^{n+1}(\mu_R^2(\{k_i\}, x_1, 2)) \delta^{LO}(a'b' \to \{k_i\}) J_{n\to n}(\{k_i\}).$$  \hspace{1cm} (4.14)

The calculation of \(d\Sigma^{z_1,z_2}/dX\) for a given \((z_1, z_2)\) amounts to doing the usual next-to-leading order calculation, with the structure functions \(f_{a'\leftarrow p}(x, Q^2)\) replaced by \(x^{-z} E_{a'a}^{z} \) (a remaining a free index), and the crossing functions \(C_{a'\leftarrow p}(x, Q^2; s_{\text{min}})\) replaced by \(x^{-z} K_{a'\leftarrow a}^{C;z} E_{a'a}^{z} \).

5. Integration Contours

The contour integrals in eqn. (3.3) must be performed numerically. This involves several distinct choices. First, we must choose an integration contour; then, we must choose a set of points along the integration contour, or in the case of hadron-hadron scattering, a set of points in the plane defined by the product of the two contours. These points must be chosen in advance, of course, so that we can evaluate the \(\Sigma\) matrices at them. How should we make these choices?
The simplest choice is to pick the textbook contour, parallel to the imaginary axis, but displaced to the right. This is what was done in the old papers of Gluck and Reya [10] on parton evolution, and also in the paper by Graudenz et al. [3]. The integral evaluated was actually \( \int_{-iT}^{c+iT} \), relying on the fall-off of the integrand as \( T \to \infty \) to drop the remaining terms. This finite-interval integral was evaluated using Gaussian quadrature. As discussed by Gluck, Reya, and Vogt [11] and in refs. [3,5], however, the integral falls off rather slowly in this direction, only as a power of the integration variable \( z \). For parton evolution, the pole structure is such that one can freely deform the contour into the left-half plane, whereupon the integrand falls off exponentially, improving the convergence of a numerical evaluation. Graudenz et al. [3] used the Mellin moments of the short-distance cross section in their formalism; these do not fall off in the left-half plane, and thus they were not able to deform the contour. (In contrast, the numerical Mellin inversions used nowadays in parton evolution programs do utilize a rotated contour [11].)

In the formalism presented in previous sections, however, the Mellin moments of the short-distance cross section appear nowhere. We may note that the experimental cuts (on rapidity and jet transverse energy) effectively impose a minimum on the parton momentum fractions \( x_{1,2} \), so that \( d\Sigma^{z_{1},z_{2}}/dX \) has no poles in the right-hand plane. Furthermore, since \( 0 < x_{1,2} < 1 \), this quantity will also fall off exponentially as \( z_{i} \to \infty \), so long as \( \text{Re} \, z_{i} < 0 \). Thus just as in refs. [11,5], we can freely shift the contour into the left-half plane, so long as we stay away from the poles of \( f_{z_{a}\to p}(Q_{0}^{2}) \) along the real axis. Indeed, much of the formalism developed in ref. [5] carries over to the choice of contours in the present paper.

The desired contour would be the contour of steepest descent (which because of analyticity is also the contour of stationary phase, upon which our integrand will be purely real). For performing the inverse Mellin transform integrals required for the evolution of parton distributions, ref. [5] shows that it is possible to construct simple but good analytic approximations to such contours, and we may hope that those findings carry over to the contours required for evaluating eqn. (3.3).

In any event, we should expect the contour of steepest descent for the leading-order calculation to be very close to that for a next-to-leading-order calculation; furthermore, we should expect it to not be very sensitive to the form of or parameters in the initial parton distributions. In practice, we have a reasonable idea of the initial distributions (the starting point for the fit, say an existing distribution set, will not be radically different from the best fit), so a good approximation to the contour of steepest descent we seek will be given by the contour of steepest descent in eqn. (3.3) for a leading-order calculation with any existing pdf set.

It will be helpful to examine first the case of lepton-hadron scattering, which is simpler because there is only one inverse Mellin transform to compute (and hence a contour in only one variable.
to choose). I shall discuss the technically more complicated hadron-hadron case in the following section. We can set up the fitting procedure following the same formalism developed in previous sections. At leading order, each iteration of a fit to a \( n \)-jet differential cross section in deeply inelastic scattering (the count excludes the remnant) requires computing

\[
\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dz \, f_{a\to p}^z(Q_0^2) \frac{d\Sigma^z_a}{dX}
\]

(with implicit summation over \( a \)), where

\[
\frac{d\Sigma^z_a}{dX} = \int_0^1 dx \int d\text{LIPS}(xk_p + k_e \to k'_e, \{k_i\}_{i=1}^n) \, x^{-z}E_{z}^{a\to a}(\alpha_s(\mu^2_F(\{k_i\}, x)), \alpha_0) \\
\times \alpha_s^{n-1}(\mu_R^2(k'_e, \{k_i\}, x_{1,2})) \delta^{1\text{LO}}(e a' \to k'_e, \{k_i\}) J_{n\to n}(\{k_i\}) \delta(X - X(k'_e, \{k_i\})).
\]

(5.1)

In principle, we could let our chosen contour depend on the variable \( X \), but this is both cumbersome and computationally more expensive. We would rather find a single contour for all values of \( X \), so long as we find a contour (along with a set of point along that contour) that yields an accurate evaluation of the integral for all \( X \) where we have data with small statistical and systematic errors. We could just take the cross section (the integral over \( X \)) but if \( X \) depends on the transverse energy \( E_T \) — that is, if the distribution is differential with respect to the transverse energy as well as other variables — then the total cross section will be dominated by events just above the lower \( E_T \) boundary. This happens because the cross section will be falling rapidly as a function of \( E_T \). It is probably better, for purposes of determining the contour, to weight the integral over \( X \) by a ‘stratifying’ function \( S(X) \) which compensates for the rapid decrease as a function of transverse energy. Take

\[
F(z) = f_{a\to p}^{0,z}(Q_0^2) \int dX \, S(X) \frac{d\Sigma^z_a}{dX},
\]

(5.2)

where \( f_{a\to p}^{0,z}(Q_0^2) \) denotes the initial parton distribution at the start of the fit procedure. We can now follow the approach outlined in ref. [5], the only change being that derivatives of \( F \) must be computed numerically rather than analytically. We can, however, write down closed-form
expressions for the required derivatives,

\[ F'(z) = \int dX S(X) \int_0^1 dx \int dLIPS(xk_p + k_e \to k_e', \{k_i\}_{i=1}^n) \times x^{-z} \left[ -\ln x E_{a' a}(\mu_F^2(\{k_i\}, x)), \alpha_0 + \frac{d}{dz} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x)), \alpha_0) \right] \times \alpha_s^{-1}(\mu_R^2(k_e', \{k_i\}, x_{1,2})) \delta^{(1)}(e' \to k_e', \{k_i\}) J_{n \to n}(\{k_i\}) \delta(X - X(k_e', \{k_i\})) \]

\[ F''(z) = \int dX S(X) \int_0^1 dx \int dLIPS(xk_p + k_e \to k_e', \{k_i\}_{i=1}^n) \times x^{-z} \left[ -2 \ln x \frac{d}{dz} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x)), \alpha_0) \right. \]

\[ \left. + \frac{d^2}{dz^2} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x)), \alpha_0) \right] \times \alpha_s^{-1}(\mu_R^2(k_e', \{k_i\}, x_{1,2})) \delta^{(1)}(e' \to k_e', \{k_i\}) J_{n \to n}(\{k_i\}) \delta(X - X(k_e', \{k_i\})) \]

\[ F^{(3)}(z) = \int dX S(X) \int_0^1 dx \int dLIPS(xk_p + k_e \to k_e', \{k_i\}_{i=1}^n) \times x^{-z} \left[ -3 \ln x E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x)), \alpha_0) + 3 \ln^2 x \frac{d^2}{dz^2} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x)), \alpha_0) \right] \]

\[ -3 \ln x \frac{d^2}{dz^2} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x)), \alpha_0) + \frac{d^3}{dz^3} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x)), \alpha_0) \right] \times \alpha_s^{-1}(\mu_R^2(k_e', \{k_i\}, x_{1,2})) \delta^{(1)}(e' \to k_e', \{k_i\}) J_{n \to n}(\{k_i\}) \delta(X - X(k_e', \{k_i\})) \].

The procedure there can be summarized as follows. First, find the minimum \( c_0 \) of \( F \) along the real axis. Next define the curve

\[ z(u) = c_0 + ic_2 \sqrt{u} + c_2^2 c_3 u/2, \]

where

\[ c_2 = \frac{\sqrt{2 F(c_0)}}{F''(c_0)}, \]

\[ c_3 = \frac{F^{(3)}(c_0)}{3 F''(c_0)}. \]

To evaluate eqn. (5.1), evaluate the transformed version,

\[ \frac{c_2}{2\pi} \int_0^\infty \frac{du}{\sqrt{u}} e^{-u} \text{Re} \left[ e^u \left( 1 - ic_2 c_3 \sqrt{u} \right) f_{a' a}^z(u) (Q_0^2) \frac{d\Sigma(z(u))}{dX} \right], \]

using a generalized Gauss-Laguerre quadrature,

\[ \int_0^\infty \frac{du}{\sqrt{u}} e^{-u} h(u) \simeq \sum_{j=1}^n w_j h(u_j^0), \]
where the \( u_j^0 \) are the zeros of the generalized Laguerre polynomial \( L_n^{(-1/2)}(u) \), and the weights are given by standard formulæ [12],

\[
w_j = \frac{\Gamma(n + 1/2)}{n! (n + 1)^2} \left[ \frac{u_j^0}{L_{n+1}^{(-1/2)}(u_j^0)} \right]^2.
\]

The number of points \( n \) required for evaluating eqn. (5.7) to a given desired precision, using the Gauss-Laguerre quadrature formula (5.8), remains to be investigated numerically, but experience with parton evolution [5] suggests that \( n \sim 5 \) should be sufficient for \(< 1\% \) error.

### 6. Contours in Hadron-Hadron Collisions

In hadron-hadron collisions, at each iteration of a fit, we have not a single contour integral to perform, but the double integral (3.3). (I again use the LO cross section to determine the contours.) Defining

\[
F(z_1, z_2) = \int_{a+p}^{0, z_1} \int_{b-p}^{0, z_2} S(X) dX d\Sigma_{ab}
\]

we have to find not an approximation to a contour of steepest descent, but an approximation to a ‘surface of steepest descent’. We can take this surface to be invariant under conjugation of each \( z_i \) separately, and use this symmetry to rewrite the contour-determining integral,

\[
-\frac{1}{4\pi^2} \int_0^{\infty} \int_0^{\infty} [dz_1 dz_2 F(z_1, z_2) - dz_1 d\bar{z}_2 F(z_1, \bar{z}_2) - d\bar{z}_1 dz_2 F(\bar{z}_1, z_2) + d\bar{z}_1 d\bar{z}_2 F(\bar{z}_1, \bar{z}_2)]
\]

\[
= -\frac{1}{2\pi^2} \int_0^{c+i\infty} \int_0^{c+i\infty} \text{Re} [dz_1 dz_2 F(z_1, z_2) - dz_1 d\bar{z}_2 F(z_1, \bar{z}_2)]
\]

(6.2)

It is not necessarily symmetric in \( z_1 \leftrightarrow z_2 \), because the beams, detector, or observable (such as a parity-violating one) may not satisfy the required \( x_1 \leftrightarrow x_2 \) symmetry.

The poles in the \( z_i \) lie along the negative real axis, so we can freely deform the contours into the left-half plane. Now just follow the procedure used in the single-contour case. First find the minimum of \( F(z_1, z_2) \) for real \( z_{1,2} \), and label its coordinates \((c_1, c_2)\). Parametrize the surface using two variables \( t_{1,2} \),

\[
\begin{align*}
z_1 &= c_1 + it_1 + a_{11} t_1^2 + a_{12} t_1 t_2, \\
z_2 &= c_2 + it_2 + a_{21} t_1 t_2 + a_{22} t_2^2.
\end{align*}
\]

(6.3)
Expand the equation \( \text{Im} F(z_1(t_1, t_2), z_2(t_1, t_2)) = 0 \) to obtain

\[
a_{11} = \frac{F^{(3,0)}}{6F^{(2,0)}}
\]
\[
a_{12} = -\frac{F^{(0,3)}}{6F^{(0,2)}} + \frac{1}{6J} \left[ F^{(0,3)} F^{(2,0)} - 3F^{(1,2)} F^{(1,1)} + 3F^{(2,1)} F^{(0,2)} - \frac{F^{(3,0)} F^{(0,2)} F^{(1,1)}}{F^{(2,0)}} \right]
\]
\[
a_{21} = -\frac{F^{(3,0)}}{6F^{(2,0)}} + \frac{1}{6J} \left[ F^{(3,0)} F^{(0,2)} - 3F^{(2,1)} F^{(1,1)} + 3F^{(1,2)} F^{(0,2)} - \frac{F^{(0,3)} F^{(2,0)} F^{(1,1)}}{F^{(0,2)}} \right]
\]
\[
a_{22} = \frac{F^{(0,3)}}{6F^{(0,2)}}
\]

where I use the abbreviated notation

\[
F^{(j_1, j_2)} = \left. \left[ \frac{\partial^{j_1+j_2} F(z_1, z_2)}{\partial z_1^{j_1} \partial z_2^{j_2}} \right] \right|_{(z_1, z_2) = (c_1, c_2)}
\]
\[
J = \det \left( \begin{array}{cc} F^{(2,0)} & F^{(1,1)} \\ F^{(1,1)} & F^{(0,2)} \end{array} \right)
\]  

(6.4)

We expect the function to go like \( F(c_1, c_2) e^{-g(t_1, t_2)} \), with

\[
g(t_1, t_2) = \frac{F^{(2,0)}}{2F(c_1, c_2)} t_1^2 + \frac{F^{(1,1)}}{F(c_1, c_2)} t_1 t_2 + \frac{F^{(2,0)}}{2F(c_1, c_2)} t_2^2
\]

(6.6)

which suggests the change of variables

\[
t_1 = \sqrt{\frac{F(c_1, c_2)(\Delta + \Lambda)}{\lambda_+ \Delta}} \sqrt{u_1} + \sqrt{\frac{F(c_1, c_2)(\Delta - \Lambda)}{\lambda_- \Delta}} \sqrt{u_2}
\]
\[
t_2 = -\sqrt{\frac{F(c_1, c_2)(\Delta - \Lambda)}{\lambda_+ \Delta}} \sqrt{u_1} + \sqrt{\frac{F(c_1, c_2)(\Delta + \Lambda)}{\lambda_- \Delta}} \sqrt{u_2}
\]

(6.7)

where

\[
\Delta = F^{(2,0)} - F^{(0,2)},
\]
\[
\lambda_{\pm} = \frac{1}{2} \left[ F^{(2,0)} + F^{(0,2)} \pm \sqrt{(F^{(2,0)} - F^{(0,2)})^2 + 4(F^{(1,1)})^2} \right]
\]

(6.8)

(6.9)

are the eigenvalues of the Hessian matrix at \( (c_1, c_2) \), and

\[
\Lambda = \lambda_+ - \lambda_-.
\]

(6.10)

Using the changes of variables (6.3,6.7), we can rewrite the integral (3.3) to be performed at each iteration of a fit as follows,

\[
\frac{1}{2\pi^2} \frac{F(c_1, c_2)}{\sqrt{J}} \int_0^\infty \int_0^\infty du_1 du_2 \frac{e^{-u_1 - u_2}}{\sqrt{u_1 u_2}} h(u_1, u_2),
\]

(6.11)
with

\[
    h(u_1, u_2) = \text{Re} \left[ e^{u_1 + u_2} (1 - i(2a_{11} + 2a_{21})u_1 - i(a_{12} + 2a_{22})u_2) \right.
\]

\[
    -2a_{11}a_{21}t_1^2(u_1) - 4a_{11}a_{22}t_1(u_1)t_2(u_2) - 2a_{12}a_{22}t_2^2(u_2) \left. \right) \times f_{\bar{a} \leftrightarrow p}(Q_0^2) f_{b \leftrightarrow \bar{p}}(Q_0^2) \int \frac{d\Sigma_{ab}(u_1, z_2(u_2))}{dx} \right] .
\]

(\(z_{1.2}\) and \(t_{1.2}\) are functions of \(u_{1.2}\) via eqns. \((6.3, 6.7)\))

We will again use the generalized Gauss-Laguerre quadrature formula, here in each of the variables \(u_i\). This would ordinarily lead to using \(n^2\) squares having chosen the \(n\)-point formula; we may note, however, that points at the far end of the square away from the origin will give a negligible contribution, so that we can restrict the sum to points \((u_0^j, u_0^k)\) with \(u_0^j + u_0^k \leq u_1^0 + u_n^0\),

\[
    \int_0^\infty \frac{du_1 du_2}{u_1 u_2} e^{-u_1 - u_2} h(u_1, u_2) \approx \sum_{j_1,j_2=1}^n w_{j_1} w_{j_2} h(u_{0}^{j_1}, u_{0}^{j_2}) \approx \sum_{\substack{j_1,j_2=1 \atop u_0^0 + u_0^j \leq u_1^0 + u_n^0}}^n w_{j_1} w_{j_2} h(u_{0}^{j_1}, u_{0}^{j_2}) .
\]

(The \(u_0^j\) are again the zeros of the generalized Laguerre polynomial \(L_n^{-1/2}(u)\), and the weights \(w_j\) are given by eqn. \((5.9)\).)

The number of points needed remains to be investigated numerically. Formulae for the various derivatives used above can be written for computer evaluation in the same fashion as in the case of deeply inelastic scattering, eqn. \((5.4)\),

\[
    \frac{\partial^{j_1 + j_2} F}{\partial z_1^{j_1} \partial z_2^{j_2}}(z_1, z_2) = f_{\bar{a} \leftrightarrow p}(Q_0^2) f_{b \leftrightarrow \bar{p}}(Q_0^2) \int dX S(X) \int_0^1 \int_0^1 dx_1 dx_2 \int d\text{LIPS}(x_1 k_p + x_2 k_{\bar{p}} \rightarrow \{k_i\}_{i=1}^n)
\]

\[
    \times \left[ x^{-z} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x_{1.2})), \alpha_0) \right] \times \frac{d^{j_1}}{dz^{j_1}} \bigg|_{z=z_1}
\]

\[
    \times \left[ x^{-z} E_{a' a}(\alpha_s(\mu_F^2(\{k_i\}, x_{1.2})), \alpha_0) \right] \times \frac{d^{j_2}}{dz^{j_2}} \bigg|_{z=z_2}
\]

\[
    \times \alpha_s(\mu_R^2(\{k_i\}, x_{1.2})) \hat{\sigma}^{LO}(a' b' \rightarrow \{k_i\}) J_{n \rightarrow n}(\{k_i\}) \delta(X - X(\{k_i\}))
\]

(\(6.14\))

where \(f_{\bar{a} \leftrightarrow p}(Q_0^2)\) denotes (as in section 5) the initial parton distribution at the start of the fit procedure.

In a practical application of the formalism presented here, one would proceed as follows. One would first determine the contours appropriate to each distribution one wanted to use in (say) fitting the parton distribution functions of the proton. (It is plausible that different distributions could make use of a common contour, but this is not guaranteed.) One would then determine the required number of points in the inversion procedure. These computations would be done using
leading-order matrix elements, as discussed above. Having chosen the points $z_{1,2}$, one would then perform a next-to-leading order computation of the quantities $d\Sigma_{ab}^{\text{LO}, \text{NLO}, \text{F}, \text{C}, \text{R}}/dX$ defined in section 4. One typically uses functional forms for the initial parton distributions whose Mellin transforms are known analytically as a function of the parameters and of the Mellin variable $z$.

One would seek to minimize the $\chi^2$ of the fit to experimental data by an iterative procedure. The Mellin transforms of the initial parton densities may be evaluated numerically for a given choice of the parameters. The quantity $h$ defined in eqn. (6.12) is then just a numerical inner product, with the ‘metric’ given by the $d\Sigma_{ab}/dX$ matrices evaluated previously. At each iteration of such a procedure, one would use eqn. (6.13) to compute the desired observable. Only the numerical values of the Mellin transforms of the initial parton densities would need to be evaluated anew at each iteration of the fit.

7. Conclusions

Jet data collected at the Tevatron and at HERA can play an important role in determining the parton distribution functions of the nucleon. To minimize renormalization-scale uncertainties, and to take full advantage of the data, they should be fitted using next-to-leading order (or higher order) theory. The formalism presented in this paper makes it computationally practical to fit to distributions culled from jet data, using a modern next-to-leading calculation. It reorganizes the calculation so that most of the time-consuming computations in an NLO program are done only once, and that each iteration of a fit involves only the recomputation of the Mellin transform of the initial parton densities at a few points, and a weighted sum over those points. The number of points required can also be minimized via choice of a quadratic contour, using the same approach detailed in ref. [5]. A similar approach could be used to reorganize the calculation of next-to-leading order corrections to allow the extraction of parton-to-hadron fragmentation functions from collider data.
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