High-precision numerical estimates of the Mellin-Barnes integrals for the structure functions based on the stationary phase contour

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Abstract. We present a recipe for constructing the efficient contour which allows one to calculate with high accuracy the Mellin-Barnes integrals, in particular, for the $F_3$ structure function written in terms of its Mellin moments. We have demonstrated that the contour of the stationary phase arising for the $F_3$ structure function tends to the finite limit as $\text{Re}(z) \to -\infty$. We show that the $Q^2$ evolution of the structure function can be represented as an integral over the contour of the stationary phase within the framework of the Picard-Lefschetz theory. The universality of the asymptotic contour of the stationary phase defined at some fixed value of the momentum transfer square $Q_0^2$ for calculations with any $Q^2$ is shown.

1 Introduction

The Mellin–Barnes (MB) integrals are widely used in high-energy physics. Their efficient numerical evaluation is an important task. The problem of finding efficient approximations of the stationary phase integration contours for the MB integrals was formulated in [1–3]. Recently, a list of studies performed using the MB integrals was supplemented by the problem of determining the structure functions and parton distributions in QCD analysis of the deep inelastic scattering (DIS) data. Significant progress in high-precision calculations of the MB integrals was achieved in the case of finite asymptotic behavior of the contour of the stationary phase at infinity [3]. The inverse Mellin transform to calculate structure functions in the Bjorken $x_B$-space, which can be considered as a typical one-dimensional integral MB, corresponds to this case. The first attempt to construct an effective approximation for the integration contour using the expansion of the integrand at the saddle point was made in [4] as applied to the calculation of parton distributions.

Here we present the basics of constructing the asymptotic contour of the stationary phase which allows one to calculate efficiently the MB integrals in the case of the finite asymptotic behavior of the contour. We also perform the studies related to the $Q^2$ evolution of the structure functions which can be done in terms of the average over the contour of the stationary phase. The dependence of the efficient integration contour on the momentum transfer squared $Q^2$ is discussed.

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2 Asymptotic contour of the stationary phase: the toy example and the structure function

In order to clarify the reason of high efficiency of a new approximation for the contour of the stationary phase, we discuss an exactly solvable example of the integration over the stationary phase contour, having a form close to that which occurs in the QCD analysis of DIS data.

The general expression for the inverse Mellin transform is written as a contour integral in the complex $z$-plane as

$$F(s) = \frac{1}{2\pi i} \int_C dz \ s^{-z} \tilde{F}(z),$$

(1)

where the contour $C$ usually runs parallel to the imaginary axis to the right of the rightmost pole. (For brevity, we omit the $Q^2$ dependence.) The function $\tilde{F}(z)$ on the right-hand side of expression (1) is the moments of the structure function usually expressed in terms of the ratio of $\Gamma$-functions. Therefore, the integral (1) is a one-dimensional MB integral.

Let us consider the simplest function

$$F(s) = s^a, \ s \in [0, 1].$$

(2)

Mellin’s moments for this function are written as

$$M(z) = \int_0^1 ds \ s^{-1} F(s) = \frac{1}{z + a} = \frac{\Gamma(a + z)}{\Gamma(a + 1 + z)}.$$

(3)

Using the inverse Mellin transform (1), we obtain

$$F(s) = \frac{1}{2\pi i} \int_{\delta - i\infty}^{\delta + i\infty} \frac{e^{uz}}{z + a}, \ u \equiv -\ln(s),$$

(4)

where the real constant $\delta$ lies to the right of all singular points $\delta > -a$.

We denote the integrand function in expression (4) as $\Phi(z)$ and consider the integration contour in the form of $z(y) = x(y) + iy$. Next, selecting the imaginary part of the $\Phi$-function and imposing the condition on the contour $\text{Im}[\Phi(z)] = 0$, we find the equation for the contour of the stationary phase $C_{st}$ as

$$[x(y) + a] \sin(uy) - y \cos(uy) = 0.$$

(5)

The solution of this equation, which provides continuity of the integration contour at the point $y = 0$, has the form

$$\begin{align*}
x_{st}(y) &= -a + y\text{ctg}(uy), \quad y \neq 0, \\
\lim_{y \to 0} x_{st}(y) &= -a + \frac{1}{u} \equiv c_0, \quad y = 0,
\end{align*}$$

(6)

(7)

where $c_0$ denotes the saddle point determined by the condition $\Phi_z(c_0) = 0$. Turning to this expression, one has for the $y(x)$

$$\begin{align*}
y(x) &= \frac{W_{st}(ux)}{u}, \\
W_{st}(ux)|_{x \to \infty} &\to \pm \pi \left[ 1 + \frac{1}{ux} + \frac{1}{(ux)^2} + O\left(\frac{1}{(ux)^3}\right) \right],
\end{align*}$$

(8)

(9)
Figure 1. The shape of efficient contours for the MB integral (4). The solid and dashed curves indicate the exact contour of the stationary phase and unshifted asymptotic contour, respectively. Horizontal lines show the asymptotics (10). The asymptotic contour after the offset to the saddle point $c_0$ (the shift is indicated by the arrow) coincides with the exact contour of the stationary phase for this example

where the generalization of the Lambert function $W_{ct}$ satisfies the transcendental equation $W_{ct}(x)\cotg[W_{ct}(x)] = x$. From (9), we find that the asymptotics of the contour $C_{st}$ is bounded and parallel to the real $x$-axis

$$y_{as} = \pm \frac{\pi}{u}.$$  \hspace{1cm} (10)

The expression (6) for the exact contour can be represented as

$$x_{st}(y) = -a + x_{as}(y),$$ \hspace{1cm} (11)

where

$$x_{as}(y) = y \cotg(u y), \quad \text{Re}(z) \rightarrow -\infty.$$ \hspace{1cm} (12)

It is clear that if the asymptotic contour, which at $y = 0$ equals to $c_{as}$, is shifted parallel to the real $x$-axis to the saddle point $c_0$, then this shifted asymptotic contour in accuracy will coincide with the contour of the stationary phase (see Fig. 1). The final expression for the asymptotic contour $C_{as}$ after the shift in the complex $z$-plane has the form

$$z_{as}(y) = x_{as}(y) + c_0 - c_{as} + iy.$$ \hspace{1cm} (13)

It is important to note that the shift according to (13) of the asymptotic integration contour to the saddle point does not change the first two terms in the expansion (9) and ensures the fast convergence if we use the quadrature formula.

To calculate the integral (4) numerically, we apply the Gauss–Legendre quadrature formula (see [3] for details). It is important that the exact contour of the stationary phase $C_{st}$, as well as the asymptotic contour $C_{as}$ have a limited asymptotic behavior as $\text{Re}(z) \rightarrow -\infty$. Using the contour $C_{as}$ defined by expression (13), we can represent the integral (4) as

$$I(s) = \int_{0}^{\left|y_{as}\right|} dy H(y),$$ \hspace{1cm} (14)

where the function $H(y)$ is given by

$$H(y) = \text{Re}\left[\left(1 - i \frac{d}{dy} x_{as}(y)\right) \Phi(z_{as}(y))\right]/\pi,$$ \hspace{1cm} (15)

and, finally, we have

$$\int_{0}^{\left|y_{as}\right|} dy H(y) \approx \frac{\left|y_{as}\right|}{2} \sum_{j=1}^{N} w_j H(y_j),$$ \hspace{1cm} (16)

\[1\] The generalization of the Lambert function $W_{ct}$ given by $W_{ct}(x)\cotg[W_{ct}(x)] = x$ was considered in [5].
where \( y_j = \frac{|y_{as}|}{2} (x_j + 1) \), \( x_j \) are the roots of the Legendre polynomials \( P_n(x) \) with normalization \( P_n(1) = 1 \), and weight coefficients \( w_j = \frac{2}{(1 - x_j^2)[P_n'(x_j)]^2} \).

The asymptotics of the contour of the stationary phase determined by expression (12) can be found without solving the equation (5), but only considering the asymptotics of the integrand in expression (4) at large-\( z \). The corresponding expression has the form: \( \Phi(z) \sim e^{u_B z} \).

Calculating the argument of the \( \Phi \)-function and equating its imaginary part to zero for \( x \to -\infty \), we arrive at the equation \( u_B y - \text{arg}(z) = 0 \) from which we get the exact expression (12).

Let us apply the described method of constructing the asymptotic contour of the stationary phase to calculate the structure function in the Bjorken variable space using the inverse Mellin transform (1). The typical parametrization of the structure function in the \( x_B \)-space (see, for example, [6]) reads for the \( F_3 \) structure function as:

\[
x_B F_3(x_B, Q^2_0) = A x_B^\alpha (1 - x_B)^\beta (1 + \gamma x_B).
\]

We can derive the Mellin moments of this structure function

\[
M_3(z) = \int_0^1 dx_B x_B^{z-1} x_B F_3(x_B) = A \left[ \frac{\Gamma(\beta+1)\Gamma(\alpha+z)}{\Gamma(\alpha+\beta+1+z)} + \frac{\Gamma(\beta+1)\Gamma(\alpha+1+z)}{\Gamma(\alpha+\beta+2+z)} \right]
\]  

(17)

and represent the structure function as the integral in the complex \( z \)-plane

\[
x_B F_3(x_B) = \frac{1}{2\pi i} \int_C dz \, \Phi^{DIS}(z), \quad \Phi^{DIS}(z) = e^{i u_B z} M_3(z), \quad u_B = -\ln(x_B).
\]  

(18)

The asymptotic behavior of the integrand \( \Phi^{DIS}(z) \) at large-\( z \) has the form

\[
\Phi^{DIS}(z) \sim e^{i u_B z} A \Gamma(\beta+1) \frac{1 + \gamma}{z^{\beta+1}}.
\]  

(19)

Based on this expression and following our method of building the asymptotic contour of the stationary phase \( C_{as} \), we find that after shifting to the saddle point \( c_0 \) this contour is expressed as

\[
z^{DIS}_{as} = y \cotg \left( \frac{u_B y}{\beta + 1} \right) + c_0 - \frac{\beta + 1}{u_B} + i y
\]  

(20)

and it has the asymptotics parallel to the real axis

\[
y^{DIS}_{as} = \pm \frac{\pi(\beta + 1)}{u_B}.
\]  

(21)

It should be noted that at \( \beta = 0 \) this expression reproduces the discussed above limit for the toy example, see expression (10).

### 3 Lefschetz thimble and \( Q^2 \) evolution of the structure function

Applying the Picard-Lefschetz theory, the inverse Mellin transform (18) for the structure function can be written in the terms of averages of the evolution factor on the Lefschetz thimble (LT) [7–12].

\[
x_B F_3(x_B, Q^2) = Z_0(\mathcal{E}^{QCD}(z, Q^2)) = \int_{\mathcal{F}(Q^2_0)} dz \mathcal{E}^{QCD}(z, Q^2) e^{-S(z)}.
\]  

(22)
\begin{table}
\centering
\begin{tabular}{cccccc}
\hline
$N$ & $C_{as}(Q_0^2)$ & $C_{as}(Q^2)$ & $C_{as}(Q_0^2)$ & $C_{as}(Q^2)$ \\
\hline
10 & $1.3 \times 10^{-4}$ & $3.4 \times 10^{-5}$ & $3.9 \times 10^{-6}$ & $1.53 \times 10^{-6}$ \\
12 & $4.1 \times 10^{-5}$ & $3.8 \times 10^{-6}$ & $1.4 \times 10^{-7}$ & $2.46 \times 10^{-8}$ \\
16 & $1.3 \times 10^{-5}$ & $4.2 \times 10^{-6}$ & $2.9 \times 10^{-10}$ & $2.4 \times 10^{-12}$ \\
20 & $3.9 \times 10^{-8}$ & $2.3 \times 10^{-9}$ & $2.2 \times 10^{-13}$ & $3.2 \times 10^{-15}$ \\
\hline
\end{tabular}
\end{table}

$$\langle E^{QCD}(z, Q^2) \rangle = \frac{1}{Z_0} \int_{\mathcal{J}(Q_0^2)} dz \, E^{QCD}(z, Q^2) \, e^{-S(z)}, \quad S(z) = -\ln(\Phi(z, Q_0^2)),$$

with the partition function

$$x_B z_0 F_3(x_B, Q_0^2) = Z_0 = \int_{\mathcal{J}(Q_0^2)} dz \, e^{-S(z)}. \quad (24)$$

The perturbative $Q^2$-evolution of the Mellin moments is well known (see, e.g., [13]), and in the non-singlet case in the leading order (LO) is given by the formula

$$M_3(z, Q^2) = M_3(z, Q_0^2) \, E^{QCD}(z, Q^2),$$

with the evolution factor

$$E^{QCD}(z, Q^2) = \exp \left[ \frac{\gamma_{as}(z)}{2\beta_0} \ln \left[ \frac{\alpha_s^{LO}(Q_0^2)}{\alpha_s^{LO}(Q^2)} \right] \right]. \quad (25)$$

The stable LT $\mathcal{J}(Q_0^2)$ is given by the path determined by

$$\dot{z} = -\partial_z S(z), \quad \partial_z S(z) \bigg|_{z=z_0} = 0, \quad (26)$$

ending at the critical point, $z_0 \in \mathcal{J}(Q_0^2)$ as the fiducial time $t \to \infty$.

The selection of the integration contour $\mathcal{J}(Q_0^2)$ in expressions (22) – (24) at the point $Q^2 = Q_0^2$ makes it universal and independent of $Q^2$. How does this influence the efficiency of calculating the structure function? The solution of the differential equation for the stationary phase contour and its subsequent application to calculate the MB integral requires big computing expenses (see, e.g., [2]). Instead of the above, it is proposed to build such approximations of the stationary phase contour that allow one to use efficient application of the quadrature integration formulae. Examples of these approximations were given in Refs. [1–4].

Returning to the discussion of $Q^2$-evolution, we consider the relative accuracy which is defined as usual $\varepsilon(N) = |[f_N - x_B F_3(x_B, Q^2)]/[x_B F_3(x_B, Q^2)]|$, where $f_N$ is the sum given by Eq. (16), when the contour $C_{as}$ (20) is used. The relative accuracy $\varepsilon(N)$ of calculating the $x_B F_3(x_B, Q^2)$ depending on the number of terms $N$ in the sums (16) is presented in Tab. 1. The result is given for $x_B = 0.01$ and $x_B = 0.5$.

Using the contour $C_{as}(Q^2)$ as the LT $\mathcal{J}(Q^2)$ approximation gives a more accurate result than using the contour $C_{as}(Q_0^2)$ as the $\mathcal{J}(Q_0^2)$ approximation. It is demonstrated in Tab. 1. This advantage is compensated by using the contour $C_{as}(Q_0^2)$ if we increase the number of terms in the quadrature formula only by 2–4 units. This is also valid for the contour approximation of the stationary phase as the parabolic contour as it was shown in [4, 14, 15].
4 Summary

We formulated a recipe for building the efficient contour which, on the one hand, has the correct behavior for $\text{Re}(z) \to -\infty$ and provides the high accuracy with growing the number terms $N$ in the quadrature formula (16), and on the other hand, this contour starts from the saddle point and provides the high accuracy for small $N$.

We have presented the inverse Mellin transformation method to evaluate $x_B$ and $Q^2$ dependences of the structure function $x_B F_3(x_B, Q^2)$ using the integration on the asymptotic contour of the stationary phase shifted to the saddle point, $C_{as}$.

When the $Q^2$-evolution of the structure function $F_3$ is taken into account, the efficiency of the contours $C_{as}(Q^2_0)$ and $C_{as}(Q^2)$ was compared. Although the contour $C_{as}(Q^2)$ gives a more accurate result, but this advantage is compensated by using the contour $C_{as}(Q^2_0)$ if we increase the number of terms in the quadrature formula only by 2–4 units. The contour $C_{as}(Q^2_0)$ can be considered as the universal one that is applicable for other values of $Q^2$. We thereby have confirmed the assumption made by Kosover for a parabolic effective contour in Ref. [4] about the universal character contour constructed with $Q^2 = Q^2_0$.

It is important to note that the computer time required to calculate the integral (18) using the quadrature formula (16) and the contour $C_{as}$ is significantly less than when using linear contours, which are as a rule parallel to the imaginary axis, to the right of the right pole in the integrand, or direct line at an angle.

The $Q^2$ evolution of the structure function $F_3$ has been represented as an integral over the contour of the stationary phase, which in the Picard-Lefschetz theory is called the Lefschetz thimble. This representation can be generalized to the singlet case and to the higher orders of the perturbation theory.

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