A new numerical method for inverse Laplace transforms used to obtain gluon distributions from the proton structure function

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We recently derived a very accurate and fast new algorithm for numerically inverting the Laplace transforms needed to obtain gluon distributions from the proton structure function $F_2^{\gamma p}(x, Q^2)$. We numerically inverted the function $g(s)$, $s$ being the variable in Laplace space, to $\tilde{G}(v)$, where $v$ is the variable in ordinary space. We have since discovered that the algorithm does not work if $g(s) \to 0$ less rapidly than $1/s$ as $s \to \infty$, e.g., as $1/s^\beta$ for $0 < \beta < 1$. In this note, we derive a new numerical algorithm for such cases, which holds for all positive and non-integer negative values of $\beta$. The new algorithm is exact if the original function $G(v)$ is given by the product of a power $v^{\beta-1}$ and a polynomial in $v$. We test the algorithm numerically for very small positive $\beta$, $\beta = 10^{-6}$ obtaining numerical results that imitate the Dirac delta function $\delta(v)$. We also devolve the published MSTW2008LO gluon distribution at virtuality $Q^2 = 5$ GeV$^2$ down to the lower virtuality $Q^2 = 1.69$ GeV$^2$. For devolution, $\beta$ is negative, giving rise to inverse Laplace transforms that are distributions and not proper functions. This requires us to introduce the concept of Hadamard Finite Part integrals, which we discuss in detail.

I. INTRODUCTION

In an earlier note [1] we developed an algorithm to numerically invert Laplace transforms in order to find an analytic solution for gluon distributions, using a global parameterization of the proton structure function, $F_2^{\gamma p}(x, Q^2)$ and a LO (leading-order) evolution equation for $F_2^{\gamma p}$. However, when we went to NLO (next-to-leading order) in the strong coupling constant $\alpha_s(Q^2)$, we have discovered the algorithm failed badly. Detailed investigation showed that the cause of the problem was that this $g(s)$—the Laplace transform of our desired NLO gluon distribution $G(v)$, where $v = \ln(1/x)$—went to 0 less rapidly than $1/s$ as $s \to \infty$, where $s$ is the Laplace space variable. The purpose of this note is to derive a new and exact algorithm for such cases, which can be modeled by Laplace transforms of the type

$$\hat{g}(s) \simeq g(s) \equiv \frac{1}{s^\beta} \sum_{k=0}^{M-1} b_k s^k,$$

(1)

for all values of positive $\beta$ and all values of non-integer negative $\beta$. We note that for $\beta = 0, -1, -2, \ldots$, the inverse Laplace transforms are the distributions $\delta(v), \delta'(v), \delta''(v), \ldots$, the Dirac delta function and its derivatives, which are not true functions but rather are distributions.

In Sections II [2] and [3] we derive exact numerical Laplace inversions for originals of the form

$$\hat{G}(v) = v^{\beta-1} \sum_{k=0}^{M-1} \frac{b_k}{\Gamma(\beta + k)} v^k,$$

(2)

but now generalized for all positive values of $\beta$ together with all negative—but non-integral—values of $\beta$. In this context, exact means calculation to arbitrary numerical precision, given a symbolic program such as Mathematica [2] which also calculates numerically to arbitrary accuracy. If the function $G(v)$ is well-approximated by $\hat{G}(v)$, one can evaluate $G(v)$ to arbitrary accuracy.

In Section IV we show that we can successfully reproduce the equivalent of a numerical delta function, using a very tiny positive $\beta$ in Eq. (1). To illustrate the new method, we will numerically invert $g(s) = 1/s^{1/1000000}$, the Laplace transform of $v^{-1+1/1000000}/\Gamma(1/1000000)$ (a numerical surrogate for a Dirac $\delta$ function) and test its accuracy.
In Section VI we solve a real physical problem, the devolution of the published LO MSTW 2008 [3] gluon distribution from the virtuality $Q^2 = 5 \text{ GeV}^2$ to $Q^2 = 1.69 \text{ GeV}^2$ (the squared mass of the $c$ quark). This calculation involves a rather large negative value of $\beta$, and consequently, calculation of a distribution, rather than a function. We must numerically compute a convolution integral in Eq. (62), i.e.,

$$
\int_0^v K_{GG}(w)\tilde{G}_0(v-w)\,dw,
$$

where the kernel $K_{GG}(w)$ is given by Eq. (2) with negative $\beta \approx -0.5$, i.e., $K_{GG}(w)$ is a distribution (not a function in the usual sense) in $w$ about half way between $\delta(w)$ and $\delta'(w)$, and thus the above integral is divergent. To obtain a convergent result, we must replace the Riemann integral sign $\int_0^v$ in Eq. (62) by the Hadamard Finite Part integral sign $\mathcal{P}$, which introduces the regularization obtained by using the Hadamard “parte finie” (Finite Part) integral [4], discussed in depth in Appendix C.

II. NUMERICAL INVERSION OF LAPLACE TRANSFORMS

Let $g(s)$ be the Laplace transform of $G(v)$. The Bromwich inversion formula for $G(v)$, which we call the original function, is given by

$$
G(v) \equiv \mathcal{L}^{-1}[g(s); v] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, g(s) e^{vs},
$$

where $c$ is a real constant such that the integration contour lies to the right of all singularities of $g(s)$. We will assume that we have made an appropriate coordinate translation in $s$ space so that those singularities all lie in the left-half complex plane, and take $c = 0$. Our goal is to numerically solve Eq. (4). The inverse Laplace transform is essentially determined by the behavior of $g(s)$ near its singularities, and thus is an ill-conditioned or ill-posed numerical problem.

In this note we present a new algorithm that takes advantage of very fast, arbitrarily high precision complex arithmetic that is possible today in programs like Mathematica [2], making the inversion problem numerically tractable.

First, we introduce a new complex variable $z \equiv vs$ and rewrite Eq. (4) as

$$
G(v) = \frac{1}{2\pi i v} \int_{-i\infty}^{+i\infty} dz \, g \left( \frac{z}{v} \right) e^{z}. \tag{5}
$$

We assume that the form of the Laplace transform $g(s)$ can be approximated as

$$
g(s) \approx \tilde{g}(s) = \frac{1}{s^\beta} \sum_{k=0}^{M-1} \frac{b_k}{s^k}, \tag{6}
$$

corresponding to an original function $G(v)$ which can be approximated as in Eq. (4) as a factor $v^{\beta-1}$ times a polynomial of order $M-1$ in $v$, i.e.,

$$
\tilde{G}(v) = \mathcal{L}^{-1}[\tilde{g}(s); v] = v^{\beta-1} \sum_{k=0}^{M-1} \frac{b_k}{\Gamma(\beta + k)} \, v^k. \tag{7}
$$

The sum contains $M$ coefficients $b_k$.

In our earlier paper [1], we proceeded to make a rational approximation for the exponential $e^z$, under the tacit assumption that $g(s)$ went to 0 sufficiently rapidly as $s$ went to $\infty$, and used this to evaluate the integral in Eq. (6). This replacement is not useful numerically if $g(s)$ goes to 0 too slowly for $s \to \pm \infty$, e.g., as $s^{-\beta}$ with $\beta < 1$ [5]. To generalize for all possible $\beta$, we now rewrite Eq. (5) as

$$
	ilde{G}(v) = \frac{1}{2\pi i v} \int_{-i\infty}^{+i\infty} dz \tilde{g} \left( \frac{z}{v} \right) z^{\beta-1} \left[ e^z \left( \frac{z}{z^{\beta-1}} \right) \right]. \tag{8}
$$

Our new algorithm uses a different treatment of the factor in square brackets.
A. The case of $\beta = 1$

In order to understand the more complicated case of $\beta \neq 1$, we briefly review here the procedure followed for the solution $\beta = 1$, detailed in Ref. [1]. When $\beta = 1$, Eq. (6) is given by

$$\tilde{g}(s) = \frac{1}{s} \sum_{k=0}^{M-1} b_k s^k$$

and Eq. (8) is given by

$$\tilde{G}(v) = \frac{1}{2\pi i v} \int_{-i\infty}^{i\infty} dz \tilde{g}\left(\frac{z}{v}\right) [e^z].$$

In the earlier paper, we approximated the square bracket $[e^z]$ by a rational function defined as a ratio of polynomials with the numerator a polynomial of order $2N - 1$ and the denominator a polynomial of order $2N$. This gives

$$[e^z] \approx \sum_{j=1}^{2N} \frac{\omega_j}{z - \alpha_j}.$$  \hspace{1cm} (11)

Inserting this into Eq. (8), using $\beta = 1$, we obtained

$$\tilde{G}(v) \approx \frac{1}{2\pi i v} \int_{-i\infty}^{i\infty} dz \tilde{g}\left(\frac{z}{v}\right) \sum_{j=1}^{2N} \frac{\omega_j}{z - \alpha_j}.$$  \hspace{1cm} (12)

The key observation for numerical purposes was that, by closing the contour of integration in the right half of the complex plane, possible with the expression in Eq. (11) but not possible for $e^z$ itself, the integral in Eq. (12) could be evaluated simply as a sum of the residues of the integrand at the poles $\alpha_j$. No numerical integration was necessary, and there were no contributions from singularities of $g(z/v)$ which lie entirely in the left half plane.

As we showed in Ref. [1], the requirement that the result be exact for all inverse powers $1/s^n$ with $1 \leq n \leq 4N$, i.e., that $M = 4N$ in Eq. (9), was sufficient to determine the $4N$ complex parameters $\alpha_i$, $\omega_i$ uniquely, and furthermore, to show that the expression in Eq. (11) was equal to the Padé approximant $P(e^z;2N-1,2N)$ of $e^z$. This is defined as the ratio of polynomials in $z$ of orders $2N-1$ and $2N$ which, when expanded, exactly reproduces the first $4N$ terms in the Maclaurin expansion of $e^z$. Conversely, the use of the $(2N-1, 2N)$ Padé approximation to $e^z$ automatically gave exact results for powers of $1/s$ in the stated range, or powers of $v$ in the original function up to $v^{4N-1}$.

The Padé approximant converges to $e^z$ to arbitrary accuracy for $N$ sufficiently large. Its use instead of $e^z$ is justified for a given $N$ if the error in the approximation to $e^z$ is sufficiently small, and $g(z/v)$ vanishes sufficiently rapidly for $s \to \pm i\infty$, that the approximation is valid over the region in $s$ that contributes significantly to the integral.

It can be shown from the properties of the Padé approximant that the poles $\alpha_j$ and weights $\omega_j$ in Eq. (11) have the following properties:

1. The poles $\alpha_j$ (the zeros of the Padé denominator) are all distinct and appear in complex conjugate pairs which we label as $(\alpha_j, \bar{\alpha}_{j+1})$, $j$ odd, with $\alpha_{j+1} = \bar{\alpha}_j$ the complex conjugate of $\alpha_j$. The poles have $\text{Re} \ \alpha_j > 0$ for all $j$, so are all in the right-hand half of the complex plane.

2. The weights $\omega_j$ also appear in complex conjugate pairs so there are $N$ distinct pairs of the complex numbers $(\omega_j, \alpha_j)$, such that the sum of the $k^{th}$ pair is real,

$$\frac{\omega_j}{z - \alpha_j} + \frac{\bar{\omega}_{j+1}}{z - \bar{\alpha}_{j+1}} \in \text{Real.} \quad j = \text{odd.}$$  \hspace{1cm} (13)

3. The integrand vanishes faster than $1/R$ as $R \to \infty$ on the semi-circle of radius $R$ that encloses the right portion of the complex plane, since the approximation vanishes as $1/R$ and $g(z/v)$ also vanishes for $R \to \infty$.

To evaluate the integral in Eq. (12) using these properties, we formed a closed contour $C$ by completing the integration path with an infinite half circle in the right portion of the complex plane, where $g(z/v)$ has no singularities. It is important to note that this contour is a clockwise path around the poles $\alpha_j$ of Eq. (12), which arise because we replaced the square bracket of Eq. (11) by $\sum_{j=1}^{2N} \omega_j/(z - \alpha_j)$. What we need is the negative of this path, i.e., the...
conjecture that the poles are to our left as we traverse the contour \(-C\). Accordingly, Eq. \([12]\) was rewritten as

\[
\hat{G}(v) = -\frac{1}{2\pi iv} \oint_{-C} \hat{g}\left(\frac{z}{v}\right) \sum_{j=1}^{2N} \frac{\omega_j}{z - \alpha_j}
\]

\[
= -\frac{1}{v} \sum_{j=1}^{2N} \frac{\alpha_j}{v} \omega_j
\]

\[
= -2 \sum_{j=1}^{N} \text{Re} \left[ \frac{\alpha_j}{v} \omega_j \right].
\]

To obtain Eq. \([15]\), we used Cauchy’s theorem to equate the closed contour integral around the path \(-C\) to \(2\pi i\) times the sum of the (complex) residues of the poles. Since the contour \(-C\) restricts us to be on the right of any singularities of \(\hat{g}(s)\), no poles of \(\hat{g}(z/v)\) are enclosed; only the \(2N\) poles \(\alpha_j\) are inside the contour. To obtain our final result for \(\hat{G}(v)\) in Eq. \([16]\), we used the properties cited above of the complex conjugate pairs in Eq. \([13]\). Taking only their real part and multiplying by \(2\), we have simultaneously insured that \(\hat{G}(v)\) is real, yet only have had to sum over half of the residues.

### B. Generalization to \(\beta \neq 1\)

The situation is more complicated for \(0 < \beta < 1\). The Laplace transform \(\hat{g}(s)\) is then of the form in Eq. \([6]\),

\[
\hat{g}(s) = \frac{1}{s^\beta} \sum_{k=0}^{M-1} b_k s^k
\]

with \(\beta\) non-integer, and the original algorithm in \([1]\) fails numerically.

To handle this case, we first rewrite the inversion formula in Eq. \([4]\) as

\[
\hat{G}(v) = \frac{1}{2\pi iv} \int_{-i\infty}^{+i\infty} dz \hat{g}\left(\frac{z}{v}\right) \left[ e^z / z^{\beta-1} \right].
\]

The function \(z^{\beta-1} \hat{g}(z)\) is of the form in Eq. \([9]\), with the original non-integer value of \(\beta\) replaced by \(1\), and causes no difficulty. The problem arises from the term in square brackets, \([\cdot] = e^z / z^{\beta-1}\). For \(\beta\) non-integer, there is no Maclaurin series about \(z = 0\), hence no Padé approximant or rational approximation for this factor.

It is still the case that the previous method works for any positive integer value of \(\beta\), \(\beta = n \geq 1\), for \(2N\) sufficiently large, a result that follows from the replacement of the first \(n - 1\) coefficients \(b_k\) in Eq. \([9]\) by zero. This suggests that the replacement of \([\cdot]\) by a rational function may still be useful for \(\beta\) non-integer. We therefore replace the bracket on the right-hand side of Eq. \([18]\) by

\[
\left[ e^z / z^{\beta-1} \right] \rightarrow \sum_{j=1}^{2N} \frac{\omega_j}{\alpha_j^{\beta-1}(z - \alpha_j)},
\]

a rational function of \(z\) which retains the form which works for integer values of \(\beta\). We stress that we do not regard this replacement as giving an adequate approximation to the term in brackets; the behavior of the two functions is quite different for \(z \rightarrow 0\) for non-integer \(\beta\).

Instead, we change our emphasis from approximation to exactness, and require that the coefficients \(\alpha_j\) and \(\omega_j\) be chosen such that the new expression gives exact results when integrated with all inverse powers \(1/s^n\) with \(1 \leq n \leq 4N\).

In the case of \(\beta = 1\), the condition of exactness required that the rational function be the Padé approximant of \(e^z\); conversely, the use of the Padé approximation for \(e^z\) led automatically to exactness. We will show here that an appropriate choice of the coefficients \(\alpha_j\) and \(\omega_j\) is possible for non-integer \(\beta\), and that the function on the right-hand side of Eq. \([19]\) is the \((2N-1, 2N)\) Padé approximant for the function \(p(z) = \Gamma(1, \beta, z) / \Gamma(\beta)\) where \(1F_1(1, \beta, z) / \Gamma(\beta)\) is the Kummer confluent hypergeometric function.

This result allows us to readily obtain exact inverse Laplace transforms for functions with \(\hat{g}(z)\) of the form in Eq. \([1]\) or Eq. \([7]\), corresponding to original functions that can be approximated by finite series of the form in Eq. \([2]\), thus justifying the seemingly arbitrary replacement \(a \text{ posteriori}\).
With this replacement, Eq. (18) can be evaluated as was done before, by closing the integration contour in the right half complex plane and using the Cauchy residue theorem, giving
\[
\tilde{G}(v) = \frac{1}{2\pi iv} \int_{-i\infty}^{+i\infty} dz \tilde{g}\left(\frac{z}{v}\right) z^{\beta-1} \frac{2N}{\alpha_j^{\beta-1}(z - \alpha_j)} \tag{20}
\]
\[
= -\frac{1}{v} \sum_{j=1}^{2N} \tilde{g}\left(\frac{\alpha_j}{v}\right) \omega_j. \tag{21}
\]

III. CANONICAL EQUATIONS

The task now is to find the appropriate \(4N\) poles \(\alpha_j\) and weights \(\omega_j\), \(j = 1, 2, \ldots, 2N\), such that the expression in Eq. (21) gives the exact inverse in Eq. (21) for all functions \(\tilde{g}(z)\) of the form in Eqs. (1) or (17). This requires that
\[
\tilde{G}(v) = v^{\beta-1} \sum_{k=0}^{2N-1} b_k \frac{\Gamma(\beta + k)}{\Gamma(\beta + k) \alpha_j^{\beta + k}} = -\frac{1}{v} \sum_{j=1}^{2N} \tilde{g}\left(\frac{\alpha_j}{v}\right) \omega_j \tag{22}
\]
\[
= -\sum_{k=0}^{2N-1} \sum_{j=1}^{2N} v^{\beta + k - 1} b_k \frac{\omega_j^{\beta + k}}{\alpha_j}. \tag{23}
\]
Equating the coefficients of the arbitrary parameters \(b_k\), we find that the \(\alpha_j\) and \(\omega_j\) must satisfy the set of 4N simultaneous equations
\[
\Gamma(\beta + k) \sum_{j=1}^{2N} \frac{\omega_j^{\beta + k}}{\alpha_j^{\beta + k}} = -1, \quad k = 0, 1, \ldots, 4N - 1. \tag{24}
\]
As is necessary, these canonical equations are independent of \(v\). The solutions of the 4N equations determine the 2N weights and 2N poles. However, the canonical equations are ill-posed for numerical purposes, so that direct solution of Eqs. (24) for weights and poles is basically impractical for even modest 2N. Fortunately, the poles and weights are readily found by other means, as will be shown in the following Section IV.

IV. DETERMINATION OF THE POLES \(\alpha_j\) AND THE WEIGHTS \(\omega_j\) FOR ARBITRARY \(\beta\)

A. Connection with Padé approximates for confluent hypergeometric functions

We will now rederive the canonical equations of Section III by a completely different technique which makes it a simple numerical task to calculate accurately and quickly the 2N poles \(\alpha_j\) and 2N weights \(\omega_j\) that satisfy the 4N canonical equations of Eq. (24).

Let us now consider a generic term of Eq. (17),
\[
\tilde{g}_k(s) = \frac{1}{s^{\beta + k}}, \quad k = 0, 1, \ldots, M - 1. \tag{25}
\]
The exact inverse Laplace transform of \(\tilde{g}_k(s)\) is given by
\[
\mathcal{L}^{-1}\left[\frac{1}{s^{\beta + k}; v = 1}\right] = \frac{1}{\Gamma(\beta + k)}, \tag{26}
\]
where, for simplicity, we have evaluated it at \(v = 1\).

We next revisit the replacement of \(e^z/z^{\beta-1}\) by a rational function which we made in Eq. (20), defining the rational function as \(\mathcal{P}(z)\),
\[
\mathcal{P}(z) = \sum_{j=1}^{2N} \frac{\omega_j}{\alpha_j^{\beta}(z - \alpha_j)}. \tag{27}
\]
This can obviously be written as the ratio of polynomials in \( z \) of orders \( 2N - 1 \) and \( 2N \) containing a total of \( 4N \) coefficients, \( 2N \) in the numerator and \( 2N \) in the denominator when the first term in the denominator is fixed to equal 1; this is just the form of a \((2N-1, 2N)\) Padé approximant.

We now rewrite Eq. (20) in terms of \( \mathcal{P}(z) \) as

\[
\tilde{G}(v) = \frac{1}{2\pi iv} \int_{-i\infty}^{i\infty} dz \tilde{g} \left( \frac{z}{v} \right) z^{-1} \mathcal{P}(z) \\
= \frac{1}{2\pi iv} \int_{-i\infty}^{i\infty} dz \tilde{g} \left( \frac{z}{v} \right) z^{-1} \left( \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k \mathcal{P}(0)}{dz^k} z^{k-1} \right),
\]

where in Eq. (29) we have substituted the Maclaurin expansion of the rational function \( \mathcal{P}(z) \).

We next examine the conditions imposed on \( \mathcal{P}(z) \) by the requirement that the result of the integration in Eq. (28) be exact for functions \( \tilde{g}(s) \) of the form in Eq. (25). When we replace \( \tilde{g}(z/v) \) by \( 1/z^{\beta+k} \) in Eq. (29) for \( v = 1 \) and close the integration contour to the left rather than the right, the result of the integration of Eq. (29) is the residue of \( \mathcal{P}(z)/z^{k+1} \) at \( z = 0 \), namely the coefficient of \( z^k \) in the Maclaurin expansion of \( \mathcal{P}(z) \) around \( z = 0 \). The condition that the result agree with the exact evaluation of the integral in Eq. (26) thus requires that

\[
\frac{1}{k!} \frac{d^k \mathcal{P}}{dz^k}(0) = \frac{1}{\Gamma(\beta+k)}, \quad k = 0, 1, 2, \ldots, 4N - 1.
\]

We can now adjust the \( 4N \) coefficients in \( \mathcal{P}(z) \) so that these conditions are satisfied for the first \( 4N \) terms in the Maclaurin expansion of \( \mathcal{P}(z) \).

Let us now extend the sum on the right hand side (r.h.s.) of Eq. (29) to infinite \( N \), and define a new function

\[
p(z) = \frac{1}{\Gamma(\beta)} \frac{z}{\Gamma(\beta+1)} + \frac{z^2}{\Gamma(\beta+2)} + \frac{z^3}{\Gamma(\beta+3)} + \cdots
\]

\[
= \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta+k)}
\]

\[
= \frac{1}{\Gamma(\beta)} {}_1F_1(1, \beta, z),
\]

where \( {}_1F_1(1, \beta, z) \) is the Kummer confluent hypergeometric function.

It is readily seen that \( \mathcal{P}(z) \) is the Padé approximant of order \((2N-1, 2N)\) for the function \( p(z) = {}_1F_1(1, \beta, z)/\Gamma(\beta) \): it is the ratio of polynomials of orders \( 2N - 1 \) and \( 2N \) which, when expanded, reproduces the first \( 4N \) terms in the Maclaurin series for \( p(z) \). This is precisely the definition of the Padé approximant for \( p(z) \), so \( \mathcal{P}(z) \equiv P(p(z), 2N-1, 2N) \). The poles \( \alpha_j \) and weights \( \omega_j, \quad j = 1, 2, \ldots, 2N \), needed for the result in Eq. (21) to be exact for \( \tilde{g}(z) \) a polynomial of degree \( 4N - 1 \) in \( 1/z \), or \( \tilde{G}(v) \) a polynomial of degree \( 4N - 1 \) in \( v \), are given by the \( 2N \) zeroes of the denominator and the \( 2N \) residues of the Padé approximant at the poles.

Although we are not aware of a formal proof except for the case \( \beta = 1 \), the poles \( \alpha_j \) are found in practice to appear only in complex conjugate pairs in the right half of the complex plane, The residues also appear in conjugate pairs. Using this information, we rewrite Eq. (21) as

\[
\tilde{G}(v) = -\frac{2}{v} \sum_{j=1}^{N} \text{Re} \left[ \tilde{g} \left( \frac{\alpha_j}{v} \right) \omega_j \right],
\]

where we sum only over the poles in the upper half plane.

We emphasize again that Eq. (34) becomes an exact statement if \( \tilde{G}(v) \) is the product of \( v^{\beta-1} \) times a polynomial of order \( 4N - 1 \). Obviously, if an original function \( G(v) \) can be adequately approximated as the product of \( v^{\beta-1} \) times a polynomial of order \( 4N - 1 \), we can then approximate \( G(v) \) by \( \tilde{G}(v) \) and write

\[
G(v) \approx -\frac{2}{v} \sum_{j=1}^{N} \text{Re} \left[ g \left( \frac{\alpha_j}{v} \right) \omega_j \right].
\]

We have found the algorithm to work very well in practice, even for fairly small values of \( 2N \).
Revisiting Eq. (19), we see that we have completely justified the replacement of the bracket by the sum for arbitrary $\beta > 0$, i.e.,

$$\left[ \frac{e^z}{z^{\beta-1}} \right] \rightarrow \sum_{j=1}^{2N} \omega_j \frac{1}{\alpha_j^{\beta-1} (z - \alpha_j)},$$  

(36)

not as an approximation for [], but as a method to obtain exact or essentially exact numerical results for a large class of functions.

We can readily calculate the $2N$ pole positions $\alpha_j$ (the zeroes of the denominator of $P(p(z), 2N - 1, 2N)$), and the $2N$ weights $\omega_j$ (the residues of $P(p(z), 2N - 1, 2N)$ at the poles) to arbitrary accuracy using a program such as Mathematica\cite{8}, which can use arbitrary-accuracy complex arithmetic.

We will show in Appendix A that the Padé approximant $P(p(z), 2N - 1, 2N)$ can actually be obtained in closed form and calculated rapidly, without the necessity of calculating $2N - 1$ fold derivatives of the function $p(z)$. As we already pointed out, since both the $\alpha_j$ and the $\omega_j$ occur in complex conjugate pairs, we only have to calculate half of them to use the relationship in Eq. (34).

A concise inversion algorithm in Mathematica that rapidly and accurately implements Eq. (16) is given in Appendix A.

Finally, we note as an aside that the function $p(z) = i F_1(1, \beta, z)/\Gamma(\beta)$ is particularly simple for some special cases. For $\beta = 1$, it becomes

$$p(z) = e^z, \quad \beta = 1,$$

(37)

and the construction above reproduces the results found in Sec. II A and [1]. For $\beta = 1/2$ and $e^z/z^{\beta-1} = z^{1/2} e^z$, the example used for illustration of a different algorithm in [6], $p(z)$ becomes

$$p(z) = z^{1/2} e^z \text{erf}(\sqrt{z}) + \frac{1}{\sqrt{\pi}} \rightarrow \infty z^{1/2} e^z; \quad \beta = 1/2,$$

(38)

where erf$(z)$ is the error function, given by erf$(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$.

More generally, the leading term in the asymptotic expansion of $p(z)$ for $\text{Re} z \rightarrow \infty$ is just $e^z/z^{\beta-1}$, the factor in square brackets in Eq. (18). However, there are additional asymptotic terms which increase less rapidly for $\text{Re} z \rightarrow \infty$. As already remarked, the behaviors of $p(z)$ and $e^z/z^{\beta-1}$ are quite different for $z \rightarrow 0$; they also differ for $z \rightarrow \pm \infty$.

### B. Analogy to Gaussian integration routines

We now slightly rewrite Eq. (34) as

$$v \tilde{G}(v) = \frac{1}{2\pi i} \int_{-i \infty}^{+i \infty} F(z) \left( \frac{e^z}{z^{\beta-1}} \right) dz \approx -2 \sum_{i=1}^{N} \text{Re} \left[ F(\alpha_i) W_i \right].$$  

(39)

where

$$F(z) = z^{\beta-1} \tilde{g} \left( \frac{z}{\nu} \right)$$  

(40)

and the weights $W_i$ are

$$W_i = \omega_i / \alpha_i^{\beta-1}.$$  

(41)

The result is exact if $F(z)$ is a polynomial in $1/z$ of degree up to $4N - 1$ because of our adjustment of the $2N$ poles $\alpha_i$ (the location of the zeroes of the Padé denominator) and the $2N$ residues $\omega_i$.

The factor $e^z/z^{\beta-1}$ in the integral of Eq. (39) evidently plays the same role in inverse Laplace transformations as the weight function $u(z)$ plays in numerical integration done by Gaussian quadrature, where the definite integral $I$ in the interval $\{-1, +1\}$ is approximated by

$$I = \int_{-1}^{+1} u(z) f(z) dz \approx \sum_{j=1}^{N} f(z_j) w_j.$$  

(42)

The $z_i$ in Eq. (12) are the $N$ zeroes of the appropriate orthogonal polynomial $P_N(z)$ in the interval $\{-1, +1\}$ for the weight function $u(z)$, and the weights $w_j$ are the Christoffel numbers of the $P_N(z_j)$. This result is exact if $f(z)$ is a polynomial of order less than or equal to $2N - 1$, since there are $2N$ coefficients, the $N$ zeroes $z_i$ and the $N$ weights $w_i$ to adjust.

With the interchange of poles and zeros, analogy between Eqs. (35) and (42) is clear.
V. A NUMERICAL APPROXIMATION OF A DIRAC DELTA FUNCTION

The Dirac delta function $\delta(v)$ is a distribution defined by its property that for any smooth test function $f(w)$,

$$\int_0^b f(v) \delta(v) dv = f(0),$$

when $b > 0$.

When $\beta = 0$ in Eq. [1], the result is $G(v) = \delta(v)$, which of course is impossible to write as a true function. We now charge our numerical Laplace inversion algorithm with the daunting task of finding an accurate numerical inversion of the Dirac delta function $\delta(v)$. We approximate it by

$$\delta(v) \approx G(v) = v^{-1+1/1000000}/\Gamma(1/1000000),$$

which uses the very tiny positive value of $\beta = 1/1000000 = 10^{-6}$ for our delta function approximation. For $f(v) = 1$, $\int_0^b G(v) dv$ is given by 0.99999 for the upper limit $b = 0.0001$ and by 1.00001 for $b = 10000$, compared to the expected value of 1, while for the test function $f(v) = \sin(v)$, the integral $\int_0^b \sin(v) G(w) dv$ is given by $1 \times 10^{-10}$ for $b = 0.0001$ and $1.6 \times 10^{-6}$ for $b = 10000$, compared to 0, thus showing that $G(v)$ is a good numerical approximation to the Dirac delta function $\delta(v)$ over an enormous range of $v$. The Laplace transform of $G(v)$ is given by

$$g(s) = \mathcal{L}[G(v;s)] = \frac{1}{s^{1/1000000}}.$$ (45)

To illustrate the accuracy of the numerical inversion routine we give in Appendix [A] we plot in Fig. [1] the numerical inversion of $g(s) = 1/s^{1/1000000}$, the Laplace transform of our numerical approximation of a $\delta$ function. The solid curve is the exact function $G(v) = v^{-1+1/1000000}/\Gamma(1/1000000)$ from Eq. [44], and the (red) dots are a result of using the algorithm in Appendix [A] using Mathematica [2]. As expected, the agreement is exact: in this case, exact means a fractional numerical precision of $O(10^{-30})$ in the entire $v$ range.

In practice, in order to use our algorithm one needs to know that the original function, the inverse Laplace transform, is well-approximated by a power law $v^{\beta-1}$ times a polynomial, as well as the numerical value of $\beta$. Normally we only have a numerical $g(s)$, so even knowing that the original function is well-approximated with a power law times a polynomial, the actual numerical value of $\beta$ is not known. However, if we can evaluate $g(s)$ numerically to arbitrary precision, we can determine $\beta$ by taking consecutive closely spaced numerical values of $g(s)$ at exceedingly large values of $s$ (thus simulating an asymptotic expansion of $g(s)$) and then fitting these numerical results to a power law in $s$. Of course, this degrades the numerical accuracy of $\beta$ considerably, but is quite viable for practical situations. For example, by fitting the function $a/s^{3\beta}$ to numerical output of Eq. [45] using 30 digit accuracy, we obtain a value for $\beta$ that is sufficiently accurate to give a relative accuracy of $O(3 \times 10^{-17})$ in inversion, more than necessary for most numerical applications. What is far more critical is knowing that the inverse transform (the original) is adequately approximated by a power law in $v$ multiplied by a finite polynomial in $v$.

VI. GLUON DEVOLUTION USING LEADING-ORDER SINGLET DGLAP EQUATIONS

In this Section we will use the work of Block, Durand, Ha and McKay [7] (BDHM), who derived analytic decoupled singlet solutions to the leading-order (LO) Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) evolution equations [8][10]. We will use their gluon solution to solve the physical problem of gluon devolution—a much more difficult problem than gluon evolution. For details of these coupled integro-differential equations and their solutions, see Ref. [2]. Here we will devolve the published LO MSTW2008LO [3] 2008 gluon distribution at the virtuality $Q^2=5$ GeV$^2$ down to $Q^2=1.69$ GeV$^2$, the square of the $c$ quark mass used by those authors.

A. Decoupled gluon solution to the LO DGLAP equation

BDHM first rewrite the standard LO singlet DGLAP equations, normally written in terms of the virtuality $Q^2$ and the variable Bjorken-$x$, in terms of new variables $v = \ln(1/x)$, $w = \ln(1/z)$. After introducing the notation $\hat{F}_s(v,Q^2) \equiv F_s(e^{-v},Q^2)$, $\hat{G}(v,Q^2) \equiv G(e^{-v},Q^2)$, they find that the singlet DGLAP equations have now been written in a form such that all of the integrals in the LO DGLAP equations are manifestly seen to be convolution integrals.
FIG. 1: A plot of the numerical Laplace inversion of $g(s) = 1/s^{1/1000000}$ and the exact original function $G(v) = v^{-1+1/1000000}/\Gamma(1000000)$ vs. $v$. The solid curve is $G(v) = v^{-1+1/1000000}/\Gamma(1/1000000)$ and the (red) dots are the numerical inversion of $1/s^{1/1000000}$, using the algorithm given in Appendix A. The fractional error of each point is $O(10^{-30})$.

Introducing Laplace transforms allows BDHM to factor these convolution integrals, since the Laplace transform of a convolution is the product of the Laplace transforms of the factors, i.e.,

$$\mathcal{L}\left[\int_0^v \hat{F}[w]H[v-w]dw; s\right] = \mathcal{L}\left[\int_0^v \hat{F}[v-w]H[w]dw; s\right] = \mathcal{L}[\hat{F}[v]; s] \times \mathcal{L}[H[v]; s].$$  (46)

Defining the Laplace transforms of $\hat{F}(v, Q^2)$ and $\hat{G}(v, Q^2)$ in Laplace space $s$ as

$$f(s, Q^2) \equiv \mathcal{L}[\hat{F}_s(v, Q^2); s] = \int_0^\infty \hat{F}_s(v, Q^2)e^{-sv} dv,$$  (47)

$$g(s, Q^2) \equiv \mathcal{L}[\hat{G}(v, Q^2); s] = \int_0^\infty \hat{G}(v, Q^2)e^{-sv} dv$$  (48)

they find two coupled first order differential equations in $Q^2$ in Laplace space $s$ that have $Q^2$-dependent coefficients, which are

$$\frac{\partial f}{\partial \ln Q^2}(s, Q^2) = \frac{\alpha_s(Q^2)}{4\pi} \Phi_f(s, Q^2) f(s, Q^2) + \frac{\alpha_s(Q^2)}{4\pi} \Theta_f(s, Q^2) g(s, Q^2),$$  (49)

$$\frac{\partial g}{\partial \ln Q^2}(s, Q^2) = \frac{\alpha_s(Q^2)}{4\pi} \Phi_g(s, Q^2) g(s, Q^2) + \frac{\alpha_s(Q^2)}{4\pi} \Theta_g(s, Q^2) f(s, Q^2).$$  (50)

The $s$-dependent coefficient functions $\Phi$ and $\Theta$ are given by

$$\Phi_f(s) = 4 - \frac{8}{3}\left(\frac{1}{s+1} + \frac{1}{s+2} + 2(\psi(s+1) + \gamma_E)\right),$$  (51)

$$\Theta_f(s) = 2n_f\left(\frac{1}{s+1} - \frac{2}{s+2} + \frac{2}{s+3}\right),$$  (52)

$$\Phi_g(s) = \frac{33-2n_f}{3} + 12\left(\frac{1}{s} - \frac{2}{s+1} + \frac{1}{s+2} - \frac{1}{s+3} - \psi(s+1) - \gamma_E\right),$$  (53)

$$\Theta_g(s) = \frac{8}{3}\left(\frac{2}{s} - \frac{2}{s+1} + \frac{1}{s+2}\right).$$  (54)
where $\psi(x)$ is the digamma function and $\gamma_E = 0.5772156\ldots$ is Euler’s constant. Here $\alpha_s(Q^2)$ is the running strong coupling constant, and for MSTW2008LO [3] is given by the LO form

$$\alpha_s(Q^2) = \frac{4\pi}{(11 - \frac{2}{3}n_f) \ln(Q^2/\Lambda^2)} \tag{55}$$

with $n_f$ the number of quark flavors. The value of the LO version of $\alpha_s$ at $Q^2 = 1$ GeV$^2$ was used in MSTW2008LO as a fitting parameter. The QCD parameters $\Lambda_3$ was adjusted to reproduce the fitted value at $Q^2 = 1$ GeV$^2$; $\Lambda_4$ and $\Lambda_5$ were fixed so that $\alpha_s$ is continuous across the boundaries at $Q^2 = M_c^2$ and $M_c^2$ where $n_f$ changes at the masses of the $b$ and $c$ quarks.

The solution of the coupled equations in Eq. (49) and Eq. (50) in terms of initial values of the functions $f$ and $g$, specified as functions of $s$ at virtuality $Q_0^2$, is straightforward. The $Q^2$ dependence of the solutions is expressed entirely through the function

$$\tau(Q^2, Q_0^2) = \frac{1}{4\pi} \int_{Q_0^2}^{Q^2} \alpha_s(Q^2) d \ln Q^2. \tag{56}$$

With the initial conditions $f_0(s) \equiv f(s, Q_0^2)$ and $g_0(s) \equiv g(s, Q_0^2)$, BDHM find the decoupled gluon solution in Laplace space $s$ is given by

$$g(s, \tau) = k_{gg}(s, \tau)g_0(s) + k_{gf}(s, \tau)f_0(s), \tag{57}$$

where the coefficient functions in the solution are

$$k_{gg}(s, \tau) = e^{\frac{6}{\alpha_s}(\Phi_f(s) + \Phi_g(s))} \left[ \cosh \left( \frac{\tau}{2} R(s) \right) - \frac{\sinh \left( \frac{\tau}{2} R(s) \right)}{R(s)} (\Phi_f(s) - \Phi_g(s)) \right], \tag{58}$$

$$k_{gf}(s, \tau) = e^{\frac{6}{\alpha_s}(\Phi_f(s) + \Phi_g(s))} \frac{2\sinh \left( \frac{\tau}{2} R(s) \right)}{R(s)} \Theta_g(s), \tag{59}$$

with $R(s) \equiv \sqrt{(\Phi_f(s) - \Phi_g(s))^2 + 4\Theta_f(s)\Theta_g(s)}$. BDHM now define two kernels $K_{GF}$ and $K_{GG}$, the inverse Laplace transforms of the $k'$s, i.e.,

$$K_{GG}(v, \tau) \equiv \mathcal{L}^{-1}[k_{gg}(s, \tau); v], \quad K_{GF}(v, \tau) \equiv \mathcal{L}^{-1}[k_{gf}(s, \tau); v]. \tag{60}$$

It is evident from Eqs. (56) and (59) that $K_{GF}$ vanishes for $Q^2 = Q_0^2$ where $\tau(Q^2, Q_0^2) = 0$. It can also be shown without difficulty that for $\tau = 0$, $K_{GG}(v, 0) = \delta(v)$ and that $K_{GF}(v, 0) = 0$.

The initial boundary conditions at $Q_0^2$ are given by $F_{s0}(x) = F_s(x, Q_0^2)$ and $G_{0}(x) = G(x, Q_0^2)$. In $v$-space, $\hat{F}_{s0}(v) \equiv F_{s0}(e^{-v})$ and $\hat{G}_{0}(v) \equiv G_{0}(e^{-v})$ are the inverse Laplace transforms of $f_0(s)$ and $g_0(s)$, respectively, i.e.,

$$\hat{F}_{s0}(v) \equiv \mathcal{L}^{-1}[f_0(s); v] \quad \text{and} \quad \hat{G}_{0}(v) \equiv \mathcal{L}^{-1}[g_0(s); v]. \tag{61}$$

Finally, BDHM writes the LO gluon distribution solution in $v$-space in terms of the convolution integrals as

$$\hat{G}(v, Q^2) = \int_0^v K_{GG}(w, \tau)\hat{G}_{0}(v-w) \, dw + \int_0^v K_{GF}(w, \tau)\hat{F}_{s0}(v-w) \, dw. \tag{62}$$

The LO gluon solution in Bjorken-$x$ space, $G(x, Q^2)$, is then easily found by going from $v$-space to $x$ space via the transformation, $G(x, Q^2) = G(\ln(1/x), Q^2)$.

### B. Devolution of the LO MSTW2008LO gluon distribution $G(x, Q^2)$ from $Q^2 = 5$ GeV$^2$ to 1.69 GeV$^2$

In order to use Eq. (62) to devolve from the leading-order MSTW2008LO gluon distribution [3] at $Q^2 = 5$ GeV$^2$ to $Q^2 = 1.69$ GeV$^2$—the MSTW value at the square of the $c$ quark mass—we must calculate the singular kernel $K_{GG}(w, \tau)$ at a negative value of $\tau$, i.e., $\tau = -0.0332005$. Asymptotically expanding $k_{gg}(s, \tau)$ in $s$ (see Eq. (58)), we can write it as

$$k_{gg}(s, \tau) \sim s^{-12\tau} e^{(33-2n_f)/3\tau}, \tag{63}$$
which shows that as \( s \to \infty \), \( k_{gg}(s, \tau) \to s^{-\beta} \), with \( \beta = 12\tau = -0.398406 \). Since \( \beta \) is negative, the kernel \( K_{GG}(w, \tau) \) in the convolution integral \( \int_0^\infty K_{GG}(w, \tau) \tilde{G}_0(v-w) \, dw \) in Eq. (62) is a distribution, and not a function. Hence, we must replace this integral with the Hadamard Finite Part integral, \( \int_0^\infty K_{GG}(w, \tau) \tilde{G}_0(v-w) \, dw \), derived in Appendix C and discussed fully there.

Using the Mathematica algorithm developed in Appendix A with \( g = k_{gg}(s, \tau) \) from Eq. (58), twob=20, beta=-0.398406, precision=100, the numerical inverse Laplace transform of the kernel \( K_{GG}(w, \tau) \) that we obtained was adequately least squares fitted—using the model of Eq. (2)—by

\[
K_{GG}(w, \tau) = \frac{w^{\beta-1}}{\Gamma(\beta)} \sum_{i=0}^{32} B_i w^i,
\]

thus determining the 33 coefficients \( B_i \). Next, we wrote the devolved gluon distribution as

\[
\hat{G}(v, Q^2 = 1.69) = \int_0^v K_{GG}(w, \tau) \tilde{G}_0(v-w) \, dw + \int_0^v K_{GF}(w, \tau) \tilde{F}_0(v-w) \, dw,
\]

evaluating the Hadamard Finite Part integral (the first integral in Eq. (63)), involving the kernel \( K_{GG} \) using the Mathematica algorithm in Appendix C while doing a straightforward evaluation of the second (Reimann) integral, using \( \beta = 1 \) in our Laplace inversion algorithm. Finally, we returned to Bjorken-\( x \) space, computing \( G(x, Q^2 = 1.69) \) using the substitution \( x = e^{-v} \).

Shown in Fig. 2 as the (red) dots are our numerical inversion devolution results for \( G(x) \) at \( Q^2 = 1.69 \text{ GeV}^2 \), devolved from \( Q^2 = 5 \text{ GeV}^2 \), compared to the published MSTW2008LO gluon distribution at \( Q^2 = 1.69 \text{ GeV}^2 \) [3]. The numerical agreement is excellent, with the fractional error at the smallest \( x \) values being \( O(1 \times 10^{-4}) \), the accuracy with which the gluon distribution is given on the Durham web site [11]. When we devolve from \( Q^2 = 10 \text{ GeV}^2 \), the fractional error becomes \( O(6 \times 10^{-4}) \); devolving from \( Q^2 = 15 \text{ GeV}^2 \), the fractional error is \( O(3 \times 10^{-3}) \); evolving from \( Q^2 = 20 \text{ GeV}^2 \), the fractional error degrades to \( O(2 \times 10^{-2}) \). The decrease in accuracy with the greater range of devolution is related to the uncertainties in the initial distributions, which are given only numerically on a grid in \( x \). The resulting uncertainties in fits to those distributions grow essentially exponentially under devolution.

VII. CONCLUSIONS

By numerically evaluating the original \( G(v) \) from the Laplace transform \( g(s) \) as

\[
G(v) = -\frac{2}{v} \sum_{i=1}^{N} \text{Re} \left[ g \left( \frac{\alpha_i}{v} \right) \omega_i \right]
\]

using the short Mathematica function given in Appendix A, we have achieved an exact numerical solution for inverse Laplace transforms whose originals are of the form

\[
G(v) = \frac{v^{\beta-1}}{\Gamma(\beta)} \sum_{i=0}^{M-1} B_i v^i, \quad M \leq 4N.
\]

When \( G(v) \) is adequately approximated by the r.h.s. of Eq. (67), we obtain an excellent numerical approximation.

We note in passing that when \( \beta = 1 \), this algorithm also replaces our earlier numerical Algorithm I [1] with a slightly more efficient one.

As an example of a very difficult numerical problem, we used the algorithm of Appendix A to invert numerically a Laplace transform of an original function which is an excellent approximation to a Dirac \( \delta \) function. We show in Fig. 1 the numerical inverse Laplace transform of \( s^{-1/1000000} \) together with the exact answer, to demonstrate the algorithm’s inherent accuracy. A fractional accuracy of \( O(10^{-30}) \) was achieved.

For our second example—a real physical problem—we accurately devolved the published MSTW2008LO gluon distribution [3] from a virtuality \( Q^2 = 5 \text{ GeV}^2 \) down to \( Q^2 = 1.69 \text{ GeV}^2 \), achieving a fractional accuracy of \( O(10^{-4}) \).

Although our inversion routine was originally developed to calculate the inverse Laplace transforms needed in work on the evolution of gluon distributions, it quite general and has a wide variety of potential applications, e.g., in the solution of both integral and differential equations.
FIG. 2: A plot of the gluon distribution $G(x)$ at $Q^2 = 1.69$ GeV$^2$ vs. Bjorken $x$. The solid curve is the published LO MSTW2008LO distribution and the (red) dots are the result of devolution from $Q_0^2 = 5$ GeV$^2$ to $Q^2 = 1.69$ GeV$^2$.

**Appendix A: A Mathematica Laplace Inversion Algorithm**

Central to this numerical algorithm is the ability to write a closed form for the Padé approximant to

$$p(z) = \frac{1}{\Gamma(\beta)} \, _1F_1(1, \beta, z),$$

which was discussed in Eq. (33).

Sidi [12], on p. 328, gives a closed form for the Padé approximant of $_1F_1(1, \beta, z)$. After some minor changes, we find that

$$P\left(\frac{_1F_1(1, \beta, z)}{\Gamma(\beta)}, 2N - 1, 2N\right) = \frac{\sum_{j=0}^{2N} (-1)^j \binom{2N}{j} \Gamma(2N + j + \beta - 1) z^{2N-j} S_{j-1}(z)}{\sum_{j=0}^{2N} (-1)^j \binom{2N}{j} \Gamma(2N + j + \beta - 1) z^{2N-j}},$$

where

$$S_j(z) \equiv \sum_{k=0}^{j} \frac{z^k}{\Gamma(\beta+k)}.$$

We now give the *Mathematica* algorithm that numerically implements Eq. (16) rapidly and accurately:

```
NInverseLaplaceTransformBlockbeta[g_, s_, v_, beta1_, twoN_, precision_] := Module[
{Omega, Alpha, M, beta, p, den, r, num, hospital},
  beta = Rationalize[beta1, 0];
  prec = Max[precision, $MachinePrecision];
  M = 2*Ceiling[twoN/2];
  Sp[p1_] := Sum[(z^j)/Gamma[beta+j], {j, 0, p1}];
  p = Expand[Sum[(-1)^j Binomial[M, j] Gamma[j+M-1+beta] z^(M-j) Sp[j-1], {j, 0, M}]]/...
```
Sum[(-1)^j Binomial[M,j] Gamma[j+M-1+beta] z^(M-j), {j,0,M}];
den=Denominator[p]; r=Roots[den==0,z]; Alpha=Table[r[[i,2]],{i,1,M}];
num=Numerator[p]; hospital=Placing[z^(-beta-1)*num/D[den,z],
Omega=SetPrecision[Table[hospital/.z->Alpha[[i]],{i,1,M,2}],prec+50];
Alpha=SetPrecision[Table[Alpha[[i]],{i,1,M,2}],prec]];
SetPrecision[-(2/v) Sum[Re[Omega[[i]]]g / s - Alpha[[i]]/v],{i,1,M/2}],prec]]

In the above algorithm, g = g(s), s = s, v = v, beta1=beta, twoN=2N in Eq. [10], and precision = desired precision of calculation. Typical values are twoN = 10−20 and precision = 30—100. The algorithm, which is quite fast, returns the numerical value of G(v).

The algorithm first insures that M=twoN is an even number. It then constructs (in closed form) p, the Padé approximant of the function 1F1(1, β, z)/Γ(β), whose numerator is a polynomial in z of order twoN-1 and whose denominator is a polynomial in z of order twoN. It then finds r, the complex roots of the denominator, which are the αi, i.e., the poles of Eq. [10]. Using L’Hospital’s rule, it finds the residue ωi corresponding to the pole αi. At this point, all of the mathematics is symbolic. It next finds every other pair (αi, ωi) to the desired numerical accuracy; they come consecutively, i.e., α1 = α2, ω1 = ω2, α3 = α4, ω3 = ω4, etc. Finally, it takes the necessary sums, again to the desired numerical accuracy, but only over half of the interval i = 1, 3, 5, …, twoN, by taking only the real part and multiplying by 2.

If g(s), the input to the algorithm, is an analytic relation and v and β are pure numbers (from the point of view of Mathematica, 31/10 is a pure number, but 3.1 is not), then, for sufficiently high values of precision, you can achieve arbitrarily high accuracy.

On the other hand, if g(s) is only known numerically, e.g., g(s) was obtained using numerical integration routines, the accuracy of inversion is limited by the need to only use relatively small values of 2N—in the neighborhood of 2−8, limiting the overall accuracy to be in the neighborhood of 10−5, which fortunately is ample for most numerical work. Typically, numerical integration routines are not accurate to better than ~10−6; one can not use ω’s—which alternate in sign—that are larger than ~1014−1016, which occur for relatively small values of 2N. Of course, this is not a limitation if g(s) is able to be expressed in closed form.

We remind the reader that the algorithm can not be used for non-positive integral values of β, because the exact inverse Laplace transforms are either the Dirac δ function or derivatives of it.

Appendix B: Comparison with similar algorithms

We had previously published two similar algorithms which we will designate as Algorithm I [1] and Algorithm II [3]. Algorithm I used the approximation

\[
\hat{G}(v) \approx \frac{1}{2\pi iv} \int_{-\infty}^{\infty} \hat{g}\left(\frac{z}{v}\right) \sum_{j=1}^{2N} \frac{\omega_j}{(z-\alpha_j)}
\]  

(B1)

and thus is identical to the present work when β = 1, as can be seen from Eq. [14]. However, the algorithm for making the Padé approximant used in Ref. [1] is a factor of ~2.5 times slower than the algorithm that we give in Appendix A. Although the majority of the computational time in both algorithms is spent in evaluating the real parts of the N complex g(αi/v), the new algorithm is slightly faster and is recommended.

Algorithm II [3] used the approximation

\[
\hat{G}(v) \approx \frac{1}{2\pi iv} \int_{-\infty}^{\infty} \hat{g}\left(\frac{z}{v}\right) \frac{1}{z^2} P(z^2e^z,2N-1,2N),
\]  

(B2)

where P(z^2e^z,2N−1,2N) is the Padé approximant of z^2e^z, whose numerator is a polynomial of order 2N−1 and whose denominator is a polynomial of order 2N. It was specifically designed to make convergent original functions such as G(v) = 1/v1−β, β < 0, and as such, required no knowledge of β. However, as suggested earlier, an accurate numerical approximation to the value of β is readily obtainable, with somewhat more effort. As an example, when using the original function G(v) = 1/\sqrt{v} of Ref. [3], the advantages of using our new algorithm is a speed factor of ~6, with a relative accuracy increase of \(O(10^{-6})\), which is a significant gain; the disadvantage is the labor to determine β. However, Algorithm II serves as a very useful numerical check that the g(s) indeed does asymptotically go as 1/s^β and that you are using an adequate numerical value for β.
Appendix C: Hadamard Finite Part Integrals

In this Section, we summarize some relevant mathematical details of (improper) Hadamard Finite Part ("parte finie") integrals, following the methods of Krommer and Ueberhuber [4], but modifying their notation somewhat after having adapted their work to our needs. We require these additional concepts when convolution integrals, such as Eq. (65), involve kernels that are not regular functions, but rather are distributions. For the convenience of the reader, we again write the devolution relation of Eq. (65), i.e.,

\[ G(v, Q^2) = \int_0^v K_{GG}(w, \tau) G_0(v - w) \, dw + \int_0^v K_{GF}(w, \tau) \hat{F}_s_0(v - w) \, dw, \quad (C1) \]

recalling that negative \( \tau \) corresponds to devolution, i.e., evolving from \( Q_0^2 \) to smaller \( Q^2 \), since \( \tau \) was defined as

\[ \tau(Q^2, Q_0^2) = \frac{1}{4\pi} \int_{Q_0^2}^{Q^2} \alpha_s(Q^2) \, d\ln Q^2, \quad \alpha_s(Q^2) > 0. \quad (C2) \]

The integral in Eq. (C1) involving the kernel \( K_{GF}(w, \tau) \to 0 \) as \( \tau \to 0 \), so it is vanishingly small for all \( w \) and presents no problems for negative \( \tau \).

However, if \( \tau \) is negative and \( |\tau| \ll 1 \), then the kernel \( K_{GG}(w, \tau) \) must be a distribution in \( w \) which is almost a \( \delta \) function, implying that it can be written as

\[ K_{GG}(w, \tau < 0) = \frac{h(w)}{w^{\beta + 1}}, \quad \beta < 0, \quad |\beta| \ll 1, \quad (C3) \]

and \( h(w) \) is a smooth polynomial in \( w \), with \( \beta \propto \tau \). Clearly, whenever the overall exponent of \( w \) is greater than 1 in the denominator of Eq. (C3), when we insert it into the first integral on the r.h.s. of Eq. (C1), the integral diverges. It is this type of divergence problem, which occurs for all negative \( \tau \) in \( K_{GG}(w, \tau) \), that we address in this Section.

1. Giving meaning to the finite portion of a divergent definite integral

To understand the concept of the Hadamard Finite Part integral, consider first the simple case of the divergent definite integral \( I_0(\beta) \) for negative \( \beta \), defined as

\[
I_0(\beta) \equiv \int_0^v \frac{1}{w^{\beta + 1}} \, dw, \quad \beta < 0, \\
= \lim_{\delta \to 0^+} \int_{\delta}^v \frac{1}{w^{\beta + 1}} \, dw \\
= \frac{1}{\beta v^{-\beta}} - \lim_{\delta \to 0^+} \frac{1}{\beta \delta^{\beta}}. \quad (C4)
\]

Equation (C4) shows that \( I_0 \) can be broken up into two parts, the finite part \( \beta^{-1}v^\beta \), which is called the Hadamard Finite Part integral, and a divergent part \( -\beta^{-1} \lim_{\delta \to 0^+} \delta^{\beta} \). It is this finite part, with \( \beta < 0 \), that is defined as the Hadamard Finite Part integral. We now introduce a new notation \( I_0^f(1/w^{\beta + 1}) \) specifically for the Hadamard Finite Part integral, now writing

\[
I_0(\beta) \equiv \int_0^v \frac{1}{w^{\beta + 1}} \, dw = \frac{1}{\beta v^{-\beta}}, \quad \beta < 0. \quad (C5)
\]

Next we generalize to a more complicated case, finding the Hadamard Finite Part integral of

\[
I_f(\beta) \equiv \int_0^v \frac{f(w)}{w^{\beta + 1}} \, dw, \quad \beta < 0, \quad (C6)
\]

where \( f(w) \) is a general (Riemann integrable) function defined on \([0, v]\). Let \( k = [\beta] \), the floor of \( -\beta \), and define \( T_k(w) \), the Maclaurin polynomial expansion of degree \( k \) of \( f(w) \) as

\[
T_k(w) = \sum_{\ell=0}^{k} \frac{f^{(\ell)}(0)}{\ell!}w^\ell. \quad (C7)
\]
Since we will require that the Hadamard Finite Part integral defined in Eq. (C6) inherit the Riemann integral properties of both linearity and additivity, we can rewrite Eq. (C6) as

\[ I_f(\beta) = \int_0^v \frac{f(w)}{w^{-\beta + 1}} \, dw = \int_0^v \frac{f(w) - T_k(w)}{w^{-\beta + 1}} \, dw + \sum_{\ell=0}^k \frac{f^{(\ell)}}{\ell!} \int_0^v \frac{1}{w^{-\beta + 1 - \ell}} \, dw. \]  

(C8)

The first integral on the right-hand side of Eq. (C8),

\[ \int_0^v \frac{f(w) - T_k(w)}{w^{-\beta + 1}} \, dw, \]  

(C9)

is readily seen to be an ordinary proper (or perhaps an improper) Riemann integral, so that we can now more simply write our definition of the finite part integral, Eq. (C8), as

\[ I_f(\beta) = \int_0^v \frac{f(w)}{w^{-\beta + 1}} \, dw = \int_0^v \frac{f(w) - T_k(w)}{w^{-\beta + 1}} \, dw + \sum_{\ell=0}^k \frac{f^{(\ell)}}{\ell!} \int_0^v \frac{1}{w^{-\beta + 1 - \ell}} \, dw, \]  

(C10)

where the only Hadamard Finite Part integrals to be evaluated are of the form

\[ \int_0^v \frac{1}{w^{-\beta + 1 - \ell}} \, dw, \quad \ell = 0, 1, \ldots, k, \quad k = [-\beta], \quad \beta < 0, \]  

(C11)

which are readily evaluated using the results of Eq. (C5).

The short Mathematica program that follows, called \texttt{intHFP[F,\{w,0,v\}],} evaluates the Hadamard Finite Part integral of Eq. (C10). For programming purposes, we have redefined the integrand \( F \) using \( F = f(w)/w^{\alpha + 1} \), whose variable \( w \) lies in \([0,v]\), i.e., we have set \( \alpha = -\beta > 0 \) in the program. Note that one can alternatively use the form \texttt{intHFP[F,\{w,0,v\},\texttt{NIntegrate}]} to do numerical integration of the integral \( \int_0^v (f(w) - T_k(w))/w^{-\beta + 1} \, dw \) when \( v \) is input as a numerical quantity, if symbolic integration is neither possible nor desirable.

\begin{verbatim}
Clear[intHFP];intHFP[F_\{f_,a_,b_,\}, int_.\texttt{Integrate}]:= Module[{f, y, \alpha, sum, k, Tk}, {f,\alpha}==F/.f_\_x^\_\alpha_.->\{f1,-\alpha\}; \alpha==\alpha-1; If[\alpha<=0,\texttt{Return}[\$Failed]]; k=If[\texttt{IntegerQ}[\alpha],\alpha-1,\texttt{Floor}[\alpha]]; If[\alpha!=0, \texttt{Return}[\texttt{Print}["Failed: Lower limit must be 0"]]]; sum=\texttt{Total@Table}[((\partial_{(\alpha)}f)/(i!))/.x->0]*(1/((\alpha-1) b^\_\alpha-.\{i,0,k\}); Tk=\texttt{Total@Table}[(\partial_{(\alpha)}f)/(i!))/.x->0] (x)^\_\alpha-. \{i,0,k\}; int[(f-Tk)/x^\_\alpha-.\{x,a,b\}+sum]; (int==\texttt{NIntegrate}||int==\texttt{Integrate}); \texttt{Clear}[x]
\end{verbatim}

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