Asymptotic Padé-Approximant Methods and QCD Current Correlation Functions

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Abstract

Asymptotic Padé-approximant methods are utilized to estimate the leading-order unknown (i.e., not-yet-calculated) contributions to the perturbative expansions of two-current QCD correlation functions obtained from scalar-channel fermion and gluon currents, as well as from vector-channel fermion currents. Such contributions to the imaginary part of each correlator are polynomials of logarithms whose coefficients (other than the constant term within the polynomial) may be extracted from prior-order contributions by use of the renormalization-group (RG) equation appropriate for each correlator. We find surprisingly good agreement between asymptotic Padé-approximant predictions and RG-determinations of such coefficients for each correlation function considered, although such agreement is seen to diminish with increasing $n_f$. The RG-determined coefficients we obtain are then utilized in conjunction with asymptotic Padé-approximant methods to predict the RG-inaccessible constant terms of the leading-order unknown contributions for all three correlators. The vector channel predictions lead to estimates for the $O(\alpha_s^4)$ contribution to $R(s) \equiv [\sigma(e^+e^- \rightarrow \text{hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)]$ for three, four, and five flavours.
1. Introduction

In phenomenological applications of perturbative QCD, one often encounters series of the form $S = 1 + R_1 x + R_2 x^2 + R_3 x^3 + \ldots$, where $x$ is the expansion parameter $\alpha_s/\pi$, and where only the first two or three coefficients $R_i$ are known. Since calculation of the higher-loop diagrams for subsequent values of $R_i$ becomes progressively more difficult, and since the expansion parameter $x$ is often large (as in QCD sum rule applications), it is important to have a reliable method of estimating subsequent radiative corrections to the series $S$ – that is, of estimating at least the first not-yet-calculated coefficient $R_i$.

In the present paper, we employ the asymptotic Padé-approximant approach (already developed to determine successfully renormalization-group functions within QCD [1,2,3] and scalar field theories [1,4]) in order to estimate the leading uncalculated contributions to the imaginary (absorptive) parts of scalar- and vector-current correlation functions within QCD. As all but nonlogarithmic terms within these contributions can be extracted by renormalization-group methods [3], the asymptotic Padé-approximant estimates for coefficients of powers of logarithms can be tested against renormalization-group predictions for these coefficients. We find an astonishing degree of accuracy in such predictions, particularly for the coefficients of the highest and next-to-highest powers of logarithms within the leading uncalculated contributions to correlators.

In Section 2, we consider the imaginary part of the scalar fermion-current correlation function, which has been calculated [5] to three subleading orders in $\alpha_s/\pi$. The fourth order term may be expressed as a degree four polynomial in $\ln(s/s_0)$, where $s_0$ is understood to be the continuum-threshold parameter of QCD sum-rule integrals in the scalar channel. We find good agreement between asymptotic Padé-approximant predictions and renormalization-group determinations for the four coefficients of $\ln^k(s/s_0) \ [k = \{1, 2, 3, 4\}]$ within the $[\alpha_s/\pi]^4$ contribution to the correlator, although this agreement diminishes as flavour-number $n_f$ increases from 3 to 6.

In Section 3, we consider the imaginary part of the scalar gluon-current correlation function, which has been calculated [6] to two subleading orders in $\alpha_s/\pi$. The leading uncalculated term is a degree-three polynomial in $\ln(s/s_0)$. Asymptotic Padé-approximant predictions for all three coefficients of $\ln^k(s/s_0) \ [k = \{1, 2, 3\}]$ are found for $n_f \leq 4$ to be in excellent agreement ($\leq 10\%$ relative error) with values determined from the renormalization group, and within $22\%$ relative error for $n_f = \{5, 6\}$.

In Section 4, the absorptive portion of the scalar fermion-current correlator is analyzed. Once again, the leading unknown contribution to this correlation function, which has been calculated to three subleading orders in $\alpha_s/\pi$ [7], is estimated by asymptotic Padé-approximant methods and compared to renormalization-group determination of the coefficients of $\ln^k(s/s_0) \ [k = \{1, 2, 3\}]$. The agreement is found to be excellent for $k = 3$ and 2, but not for $k = 1$, where an approximate factor-of-two discrepancy is seen to occur. This discrepancy is explored further by expressing the asymptotic Padé-approximant estimate for the leading unknown contribution to the vector correlator as an asymptotic series in the variable $L \equiv -\ln(s/s_0)$: $R_4 = d_3 L^3 + d_2 L^2 + d_1 L + \ldots$. The two leading series coefficients $d_{3,2}$ of this large-L expansion replicate exactly the renormalization-group determination of the two leading polynomial coefficients $d_{3,2}$ within the $R_4$ contribution to the vector correlator, i.e., the coefficients of $-\ln^3(s/s_0)$ and $\ln^2(s/s_0)$. The coefficient $d_1$ of $-\ln(s/s_0)$ obtained from this large-L expansion, corresponding to an alternative Padé-approximate estimate of the $k = 1$ coefficient, is found to differ substantially from the correct value. However, these two asymptotic Padé-approximant approaches for estimating the $k = 1$ coefficient, as delineated above, are seen to straddle the correct result, suggesting for the vector correlator an overall insensitivity of asymptotic Padé-approximant methods to the $k = 1$ coefficient. A least-squares determination of the coefficients $d_k$ confirms this insensitivity to $d_1$.

Finally, in Section 5 we utilize asymptotic Padé-approximant methods, in conjunction with renormalization-group determinations of $\ln^k(s/s_0)$ polynomial coefficients, in order to estimate those constant (i.e., $k = 0$) terms which cannot at present be extracted by renormalization-group methods. Such terms are of phenomenological interest for estimating higher-loop effects in QCD Laplace and finite-energy sum-rules. Moreover, such predictions can be tested against subsequent perturbative calculations. Of particular interest are predictions obtained for the $O(\alpha_s^4)$ term in $R(s) \equiv \sigma(e^+ e^- \rightarrow hadrons)/\sigma(e^+ e^- \rightarrow \mu^+ \mu^-)$. 

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2. The Scalar Correlator for Fermion Currents

We consider first the scalar current correlation function

\[ \Pi_s(p^2) = i \int d^4y e^{ip\cdot y} <0|T_j_s(y)j_s(0)|0> \]  

(2.1)

based upon the scalar fermion current

\[ j_s(y) = \bar{\psi}(y)\psi(y) \]  

(2.2)

The absorptive portion of this correlator may be expressed in terms of the ratio \( w \equiv s/s_0 \), where \( s \equiv p^2 \), and \( s_0 \) is the continuum threshold usual to QCD sum-rule analysis (i.e., the kinematic threshold above which purely-perturbative QCD alone is adequate to describe the correlation function):

\[
\frac{1}{\pi} \text{Im} \Pi_s = \frac{3s}{8\pi^2} \left[ 1 + \frac{\alpha_s(s_0)}{\pi} R_1(w) + \left( \frac{\alpha_s(s_0)}{\pi} \right)^2 R_2(w) + \left( \frac{\alpha_s(s_0)}{\pi} \right)^3 R_3(w) + \left( \frac{\alpha_s(s_0)}{\pi} \right)^4 R_4(w) + \ldots \right]
\]  

(2.3)

The coefficients \( R_1(w) \), \( R_2(w) \) and \( R_3(w) \) have been determined for arbitrary flavour number [5]. For example, when \( n_f = 3 \), these are given by

\[ R_1(w) = 17/3 - 2\ln(w) \]  

(2.4)

\[ R_2(w) = 31.8640 - (95/3)\ln w + (17/4)(\ln w)^2 \]  

(2.5)

\[ R_3(w) = 89.1564 - 297.596\ln w + (229/2)(\ln w)^2 - (221/24)(\ln w)^3. \]  

(2.6)

This information is sufficient in itself to generate an asymptotic Padé-approximant prediction for \( R_4(w) \) [3,4]:

\[
R_4(w) = \frac{R_2^2(w) [R_3^2(w) + R_1(w)R_2(w)R_3(w) - 2R_1^2(w)R_3(w)]}{R_2^2(w)[2R_3^2(w) - R_1^2(w)R_3(w) - R_1^2(w)R_2^2(w)]}
\]  

(2.7)

This prediction, in turn, may be utilized to generate (via numerical integration) the first five (nonsingular) finite-energy-sum-rule moments [4]

\[ N_k \equiv (k+2) \int_0^1 dw w^{k+1} R_4(w) \]  

(2.8)

of the \( O(\alpha_s^4) \) contribution to the scalar correlation function. Substituting (2.7) into (2.8), we find that

\[ N_{-1} = 7544.9, \ N_0 = 2059.4, \ N_1 = 1158.4, \ N_2 = 833.47, \ N_3 = 673.29 \]  

(2.9)

The significance of these moments is that they may be used to estimate the polynomial coefficients of \( \ln(w) \) in \( R_4(w) \), which is known to be fourth-order in \( \ln w \):

\[ R_4(w) = d_0 - d_1 \ln w + d_2(\ln w)^2 - d_3(\ln w)^3 + d_4(\ln w)^4; \]  

(2.10)

Substituting (2.10) into (2.8) we see that

\[ N_{-1} = d_0 + d_1 + 2d_2 + 6d_3 + 24d_4 \]  

(2.11)

\[ N_0 = d_0 + d_1/2 + 2d_2/2 + 3d_3/4 + 3d_4/2 \]  

(2.12)

\[ N_1 = d_0 + d_1/3 + 2d_2/9 + 2d_3/9 + 8d_4/27 \]  

(2.13)

\[ N_2 = d_0 + d_1/4 + 2d_2/8 + 3d_3/32 + 3d_4/32 \]  

(2.14)
The agreement between these numbers and the asymptotic Padé predictions (2.16) is astonishing close, ranging from eqs. (2.22-25) the following RG determination of the

\[ O(\alpha_s^4) \]

coefficients \( d_1 - d_4 \). Their solution is

\[ d_0 = 252.5, \quad d_1 = 1339, \quad d_2 = 1695, \quad d_3 = 345.7, \quad d_4 = 20.38 \]  

(2.16)

The exact values for the coefficients \( d_1 - d_4 \) may be extracted [4] from the renormalization group equation (RG)

\[
0 = \left[ s_0 \frac{\partial}{\partial s_0} + \beta(x) \frac{\partial}{\partial x} + 2\gamma_m(x) \right] \text{Im}\Pi(L(s_0), x); \\
x = \alpha_s/\pi; \quad L(s_0) \equiv \ln(s_0/s) = -\ln w; \quad \left( s_0 \frac{\partial}{\partial s_0} = \frac{\partial}{\partial L} \right)
\]

(2.17)

As is evident from (2.3) and (2.4-6), the correlation function is in the following form

\[
\text{Im}\Pi(L, x) = \frac{3\pi}{8\pi}(1 + (a_0 + a_1 L)x \\
+ (b_0 + b_1 L + b_2 L^2)x^2 + (c_0 + c_1 L + c_2 L^2 + c_3 L^3)x^3 \\
+ (d_0 + d_1 L + d_2 L^2 + d_3 L^3 + d_4 L^4)x^4 + \ldots)
\]

(2.19)

where \( a_i, b_i, c_i \) are given in eqs. (2.4-6):

\[ a_0 = 5.66667, \quad a_1 = 2, \quad b_0 = 31.8640, \quad b_1 = 31.6667, \quad b_2 = 4.25 \]
\[ c_0 = 89.1564, \quad c_1 = 297.596, \quad c_2 = 114.5, \quad c_3 = 9.20833 \]

(2.26)

For \( n_f = 3 \) the values of \( a_i, b_i, c_i \) are given in eqs. (2.4-6):

\[ a_0 = 5.66667, \quad a_1 = 2, \quad b_0 = 31.8640, \quad b_1 = 31.6667, \quad b_2 = 4.25 \]
\[ c_0 = 89.1564, \quad c_1 = 297.596, \quad c_2 = 114.5, \quad c_3 = 9.20833 \]

(2.26)

Corresponding values for \( \beta_i \) and \( \gamma_i \) are [8]

\[ \beta_0 = 2.25, \quad \beta_1 = 4, \quad \beta_2 = 10.0599, \]
\[ \gamma_1 = 3.79166, \quad \gamma_2 = 12.42018, \quad \gamma_3 = 44.2628. \]

(2.27)

One then obtains from eqs. (2.22-25) the following RG determination of the \( O(\alpha_s^4) \) coefficients \( d_1 - d_4 \):

\[ d_1 = 1563.0, \quad d_2 = 1583.6, \quad d_3 = 356.04, \quad d_4 = 20.143. \]

(2.28)

The agreement between these numbers and the asymptotic Padé predictions (2.16) is astonishing close, ranging from a 14% relative error in the prediction of \( d_1 \) to a 1.2% error in the prediction of \( d_4 \). This close agreement supports the two-parameter asymptotic error formula [3]

\[
\delta_{N+2} \equiv \frac{R_{N+2}^{[N+1]} - R_{N+2}}{R_{N+2}} = -\frac{A}{N + 1 + B}
\]

(2.29)

used to derive the asymptotic Padé-approximant prediction (2.7) in ref [4].

The above agreement is not peculiar to \( n_f = 3 \). Table 3 tabulates corresponding results for the \( n_f = 4, 5 \) and \( 6 \) scalar-correlation functions. It is evident from Table 3 that the accuracy of asymptotic Padé-approximant predictions for \( d_1 - d_4 \) is actually better for \( n_f = 4 \) and 5 than it is for \( n_f = 3 \). A diminution of accuracy becomes evident only when \( n_f = 6 \).
3. The Scalar Correlator for Gluon Currents

We now consider the QCD gluonic scalar current correlation function $\Pi_G = \langle \frac{\beta(\alpha_s/\pi)G^2}{\alpha_s\beta_0} \rangle$. This correlation function is of the same form as (2.1) but with $j_s(y)$ replaced with the RG-invariant gluonic current $j_G(y)$

$$j_s(y) \rightarrow j_G(y) = \frac{\beta(\alpha_s/\pi)}{\alpha_s\beta_0} c_\mu \rho'(y) G^{\frac{4}{3}w}(y)$$ (3.1)

The absorptive portion of this correlation function can be extracted to order-$\alpha_s^3$ from a previous three-loop calculation [6] of the correlation function $\langle (G^2)^2 \rangle$. Using our previous notation we find that

$$Im \Pi_G(L, x) = \frac{x^2}{\pi^2 x_0^2} [\beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3]^2 Im \langle (G^2)^2 \rangle$$

$$= \frac{2x^2 s^2}{\pi^3} [1 + (a_0 + a_1 L)x$$

$$+ (b_0 + b_1 L + b_2 L^2)x^2$$

$$+ (c_0 + c_1 L + c_2 L^2 + c_3 L^3)x^3 + ...]$$ (3.2)

where $x \equiv \alpha_s/\pi$ and $L \equiv ln(s_0/s)$, as before, and where the known coefficients $a_0, a_1, b_0, b_1$, and $b_2$ are tabulated in Table 4. These coefficients are sufficient in themselves to determine the aggregate coefficients of $x$ and $x^2$ in the correlator:

$$R_1(w) = a_0 - a_1 ln w,$$ (3.3)

$$R_2(w) = b_0 - b_1 ln w + b_2 [ln(w)]^2,$$ (3.4)

$$Im \Pi_G = \frac{2x^2 s^2}{\pi^3} [1 + xR_1(w) + x^2R_2(w) + x^3R_3(w) + ...] .$$ (3.5)

Asymptotic Padé-approximant methods may be utilized to predict that [4]

$$R_3(w) = \frac{2R_3^2(w)}{R_1^2(w) + R_1(w)R_2(w)} .$$ (3.6)

This function may then be employed in the integrands of moment integrals

$$P_k = (k + 1) \int_0^1 dw w^k R_3(w)$$ (3.7)

for $k = \{0, 1, 2, 3\}$. The numerical values of $P_k$ can then be used, as before, to determine explicitly the coefficients $c_{0,1,2,3}$ that characterize $R_3(w)$ as a degree-3 polynomial in $ln(w)$:

$$R_3(w) = c_0 - c_1 ln w + c_2 (ln w)^2 - c_3 (ln w)^3,$$ (3.8)

$$P_0 = c_0 + c_1 + 2 c_2 + 6 c_3$$ (3.9)

$$P_1 = c_0 + c_1/2 + c_2/2 + 3 c_3/4$$ (3.10)

$$P_2 = c_0 + c_1/3 + 2 c_2/9 + 2 c_3/9$$ (3.11)

$$P_3 = c_0 + c_1/4 + c_2/8 + 3 c_3/32$$ (3.12)

In Table 4, the values of these integrals $P_k$ are tabulated for $n_f = \{0, 2, 3, 4, 5, 6\}$, as extracted via (3.6) from (3.3) and (3.4). These integrals, in turn, are sufficient to predict the coefficients $\{c_0, c_1, c_2, c_3\}$ by explicit solution of the set of linear equations (3.9 - 12). These predicted values of $c_{0-3}$ are labelled as asymptotic Padé-approximant predictions (APAP) and tabulated at the bottom of Table 4.
As in the previous section, all but one \( (c_0) \) of these coefficients may be extracted via the renormalization-group equation satisfied by the gluonic scalar-current correlation function
\[
\left( \frac{\partial}{\partial L} + \beta(x) \frac{\partial}{\partial x} \right) \text{Im} \Pi_G(L,x) = 0,
\]
where, as before, \( \partial/\partial L = s_0 \partial/\partial s_0 \), and where \( \beta(x) \) is given by (2.20) with the coefficients listed in Table 2. Upon application of (3.13) to the explicit form (3.2) for \( \text{Im} \Pi_G \), one finds that
\[
c_1 = 2\beta_2 + 3\beta_1 a_0 + 4\beta_0 b_0 \quad (3.14)
\]
\[
2c_2 = 3\beta_1 a_1 + 4\beta_0 b_1 \quad (3.15)
\]
\[
3c_3 = 4\beta_0 b_2. \quad (3.16)
\]
We have tabulated values of \( c_1, c_2, c_3 \) extracted via these equations as \( c_1^{(RGE)}, c_2^{(RGE)} \) and \( c_3^{(RGE)} \) towards the bottom of Table 4. In comparing asymptotic Padé-approximant predictions (APAP) for \( c_{1-3} \) to their actual values, as determined from RG (3.13), one finds accuracy within 4% for \( c_1 \) and \( c_2 \), and within 6% for \( c_3 \) when \( n_f = 0 \). This accuracy diminishes somewhat as \( n_f \) increases, although the agreement remains striking even out to six flavours. Table 4’s least accurate asymptotic Padé-approximant prediction, that of \( c_1 \) when \( n_f = 6 \), differs from the true (RG) value by only a 22% relative error. This agreement may be understood to confirm the applicability of the one-parameter simplification of the asymptotic error formula (2.29)
\[
\delta_{N+2} = -\frac{A}{N+1} \quad (3.17)
\]
obtained in ref. [1] and utilized in Section 5 of ref. [4] to obtain eq. (3.6).

4. The Vector Correlator for Fermion Currents

The vector-current correlation functions may be extracted from the Adler-function (“D-function”) presented in ref [7]:
\[
\Pi_v(Q^2) = \frac{4}{3} \sum_f Q_f^2 \left\{ \ln \left( \frac{Q^2}{\mu^2} \right) (1 + x) \right.
\]
\[
+ x^2 \left[ A_0 \ln \left( \frac{Q^2}{\mu^2} \right) + A_1 \left( \ln \left( \frac{Q^2}{\mu^2} \right) \right)^2 \right]
\]
\[
+ x^3 \left[ B_0 \ln \left( \frac{Q^2}{\mu^2} \right) + B_1 \left( \ln \left( \frac{Q^2}{\mu^2} \right) \right)^2 + B_2 \left( \ln \left( \frac{Q^2}{\mu^2} \right) \right)^3 \right]
\]
\[
+ \mathcal{O}(x^4) \} \quad (4.1)
\]
where \( x = \alpha_s/\pi \), as before, and where [7]
\[
A_0 = 1.98571 - 0.115295n_f \quad (4.2)
\]
\[
A_1 = -1.375 + 0.0833333n_f \quad (4.3)
\]
\[
B_0 = -1.23954(\sum_f Q_f)^2/[3 \sum_f Q_f^2] + 18.2427 - 4.21585n_f + 0.0862069n_f^2 \quad (4.4)
\]
\[
B_1 = -8.64820 + 1.04385n_f - 0.0192159n_f^2 \quad (4.5)
\]
\[
B_2 = 2.52083 - 0.305556n_f + 0.00925926n_f^2 \quad (4.6)
\]
If we identify $\mu^2$ with the continuum threshold $s_0$, we find that the absorptive portion of this correlator is given by

$$\frac{1}{\pi} Im \Pi_v = -\frac{4}{3} \sum_f Q_f^2 \left[ 1 + xR_1(w) + x^2R_2(w) + x^3R_3(w) + x^4R_4(w) \ldots \right]$$  
(4.7)

where $w \equiv s/s_0$ and where

$$R_1(w) = 1$$  
(4.8)
$$R_2(w) = A_0 - (-2A_1)\ln w$$  
(4.9)
$$R_3(w) = (B_0 - \pi^2B_2) - (-2B_1)\ln w + 3B_2(\ln w)^2.$$  
(4.10)

With this information, it is possible to repeat the calculation of Section 2 in order to estimate the $O(x^4)$ coefficients within $Im \Pi_v$. One can utilize (4.8), (4.9) and (4.10) within (2.7) to obtain an asymptotic Padé-approximant prediction of the function $R_4(w)$. Using this function, one can explicitly evaluate the moment integrals $N_{-1}$, $N_0$, $N_1$, and $N_2$, as defined by eq. (2.8). These four moments are sufficient to provide an estimate of the polynomial coefficients $d_i$ within $R_4(w)$, which must be degree-3 in $\ln w$:

$$R_4(w) = d_0 - d_1\ln w + d_2(\ln w)^2 - d_3(\ln w)^3.$$  
(4.11)

The four linear equations relating moment integrals $N_k$ to coefficients $d_i$ are given by (2.11-14), with the constant $d_i$ taken to be zero [the corresponding $x^4$ term for the scalar correlator was degree-4 in $\ln w$]. These four equations can then be solved to obtain asymptotic Padé-approximant (APAP) estimates of $d_0$, $d_1$, $d_2$, and $d_3$.

We have tabulated these estimates for $n_f = \{2, 3, 4, 5\}$ in Table 5. These estimated values for $d_1-3$ can be tested against renormalization group determinations of these coefficients. The vector-current correlation function (4.7) can be parametrized similar to $\Pi_G(L, x)$ in (3.2):

$$\frac{1}{\pi} Im \Pi_v(L, x) = -\frac{4}{3} \sum_f Q_f^2 \left[ 1 + x + (b_0 + b_1L)x^2 + (c_0 + c_1L + c_2L^2)x^3 \right.$$  
$$+ \left. (d_0 + d_1L + d_2L^2 + d_3L^3)x^4 \ldots \right]$$  
(4.12)

where $L \equiv \ln(s_0/s) = -\ln w$, and where the constants in (4.12) are related to those in (4.1) by

$$b_0 = A_0, \ b_1 = -2A_1, \ c_0 = B_0 - \pi^2B_2, \ c_1 = -2B_1, \ c_2 = 3B_2.$$  
(4.13)

The correlator (4.12) has the same RG-invariance as (3.2), and is therefore a solution of (3.13). This equation predicts the following values for $d_1$, $d_2$, and $d_3$:

$$d_1 = 3\beta_0c_0 + 2\beta_1b_0 + \beta_2$$  
(4.14)
$$d_2 = (3\beta_0c_1 + 2\beta_1b_1)/2$$  
(4.15)
$$d_3 = \beta_0c_2.$$  
(4.16)

On can further show via (3.13) [or explicitly from substituting (4.2-5) into (4.13)] that

$$b_1 = \beta_0, \ c_1 = 2\beta_0b_0 + \beta_1, \ c_2 = \beta_0^2$$  
(4.17)

in which case

$$d_2 = 3\beta_0^2b_0 + \frac{5}{2}\beta_0\beta_1, \ d_3 = \beta_0^3.$$  
(4.18)

Table 5 displays RG determinations of $d_1$, $d_2$, $d_3$ immediately below their APAP estimates. Striking agreement is evident from the Table between APAP and RG estimates of $d_3$ and $d_2$ for $n_f = \{2, 3\}$, an agreement which
deteriorates as \( n_f \) increases. However, the APAP estimates of \( d_1 \) seem to be a factor of two too large across the entire set of flavours considered.

This discrepancy, however, is more indicative of insensitivity of APAP methods to the value of \( d_1 \) and \( d_0 \) for the vector correlator case, rather than of any overall failure of APAP methodology, as epitomized by eq. (2.7). Indeed, if we use eq. (2.7) directly (as opposed to the moment integrals \( N_b \)) to predict \( d_3 \), \( d_2 \), \( d_1 \) and \( d_0 \), we not only obtain much different values for \( d_1 \), but also results identical to the RG determinations of \( d_2 \) and \( d_3 \). To see this, consider the large-L asymptotic expansion of (2.7), with \( R_{1-4} \) as parametrized in (4.12) \([R_1 = 1, R_2 = b_0 + b_1L, R_3 = c_0 + c_1L + c_2L^2]\):

\[
R_4 = \left[ \frac{c_1^2(b_0^2 + c_2)}{2b_1^2} \right] L^3 + \left[ \frac{c_1^2}{4b_1^2} - \frac{[c_1^2(1 + 3b_0)]}{2b_1^2} \right] + \frac{3c_1c_2^2}{2b_1^2} + \left[ \frac{c_2^2(1 - 2b_0)}{4b_1^2} + c_1c_2 \right] L^2 + \mathcal{O}(L)
\]

\[
= d_3^{APAP'} L^3 + d_2^{APAP'} L^2 + d_1^{APAP'} L + ...
\]

Using (4.17) within the first two terms listed in (4.19), we find that

\[
d_3^{APAP'} = \beta_0^3,
\]

\[
d_2^{APAP'} = 3\beta_0^2b_0 + 5\beta_0\beta_1/2.
\]

These APAP’ predictions, based entirely upon (2.7), coincide exactly with the RG determinations (4.18) of \( d_3 \) and \( d_2 \). In Table 6 we tabulate the corresponding predictions \( d_1^{APAP'} \), as obtained via the large-L expansion (4.19), for the coefficient \( d_1 \). Also tabulated are the prior (APAP) predictions of \( d_1 \) obtained via use of (2.7) within the integrands of moment integrals \( N_b \), along with renormalization-group (RG) determinations of \( d_1 \). As is evident from the Table, the true (RG) value of \( d_1 \) is straddled by the two Padé predictions, demonstrating the insensitivity of Padé methodology to \( d_1 \), the “sub-subleading” \( \mathcal{O}(x^3) \) coefficient in the vector channel.

This insensitivity of the \( d_1 \) prediction is evident from a least-squares approach which finds values for \( d_k \) which minimize the quantity

\[
\chi^2(d_0, d_1, d_2, d_3) = \int_0^1 [R_4(w) - (d_0 - d_1 \log(w) + d_2 \log^2(w) - d_3 \log^3(w))]^2 dw
\]

where \( R_4(w) \) is obtained by substituting (4.8-10) into (2.7). For \( n_f = 3 \), the \( \chi^2 \) integral (numerically evaluated) becomes the following quadratic form:

\[
\chi^2(d_0, d_1, d_2, d_3) = 227586.642 + 720d_2^2 + 12d_3d_0 + 24d_2^2 + 48d_1d_3 + 2d_2^3 + 240d_2d_3 + d_0^2 + 12d_1d_2 + 2d_1d_3 + 4d_2d_0 - 237.6405798d_0 - 908.3757480d_1 - 4402.296530d_1 - 25479.03758d_3
\]

Minimization of the \( \chi^2 \) is equivalent to minimization of the matrix quadratic form

\[
(Ax - b)^2
\]

where

\[
x = \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \end{pmatrix}, \quad A = \begin{pmatrix} 2 & 2 & 4 & 12 \\ 2 & 4 & 12 & 48 \\ 4 & 12 & 48 & 240 \\ 12 & 48 & 240 & 1440 \end{pmatrix}, \quad b = \begin{pmatrix} 237.6405798 \\ 908.3757480 \\ 4402.296530 \\ 25479.03758 \end{pmatrix}
\]

The singular value decomposition of \( A \) is

\[
A = U\Sigma V^T, \quad \Sigma = \sigma_i\delta_{ij}
\]

\[
\sigma_0 = 1481.970038, \quad \sigma_1 = 10.52846941, \quad \sigma_2 = 1.395692455, \quad \sigma_3 = 0.105800579
\]

\[
U = \begin{pmatrix} -0.008483667052 & -0.2757146361 & 0.8783851152 & -0.3903191722 \\ -0.03336418987 & -0.4565091835 & 0.2371489578 & 0.856818869 \\ -0.1652682630 & -0.8311862313 & -0.4115179052 & -0.335367783 \\ -0.9856476345 & 0.1571949543 & 0.05341324608 & 0.03058614050 \end{pmatrix}
\]

\[
V = \begin{pmatrix} 0.510683712 & 0.725953393 & 0.179634106 & -0.541366246 \\ -0.280002728 & 0.418397125 & 0.713440646 & -0.222064734 \\ -0.215995328 & 0.534399698 & -0.722873585 & 0.237018473 \\ -0.727878008 & -0.214146011 & 0.173097864 & 0.718412160 \end{pmatrix}
\]
and the quadratic form becomes

\[(Ax - b)^2 = (\Sigma y - b')^2 = \sum_{i=0}^{3} (\sigma_i y_i - b'_i)^2 , \quad b' = U^T b , \quad y = V^T x \]  \tag{4.29}\]

Although the quadratic form (and \(\chi^2\)) is minimized by

\[y_i = \frac{b'_i}{\sigma_i} \implies y_0 = -17.4587 , \quad y_1 = -12.7421 , \quad y_2 = -19.0195 , \quad y_3 = -108.2255 \]  \tag{4.30}\]

the wide range of singular values \(\sigma_0 \gg \sigma_2 > \sigma_3\) implies that the \(\chi^2\) depends strongly on \(y_0\) and \(y_1\), but is relatively insensitive to \(y_2\) and \(y_3\). This broad \(\chi^2\) minimum in the \(y_2\) and \(y_3\) directions compared with the sharp minimum in the \(y_0\) and \(y_1\) directions implies a comparatively large uncertainty in the extraction of \(y_2\) and \(y_3\) from the Padé approximation. Since \(y_3\) is both large and uncertain, the relation \(x = V y\) implies that \(d_0\) and \(d_1\) (and to a lesser extent \(d_2\)) are dominated by the values of \(y_2\) and \(y_3\) rather than \(y_0\) and \(y_1\), and hence \(d_0, d_1\) are poorly determined. However, the \(y_2, y_3\) dependence of the RG accessible \(d_k\) can be eliminated to find the single linear combination independent of \(d_0\) that is well determined by the \(\chi^2\) minimization:

\[d_3 + 0.01950310416 d_1 + 0.1410349007 d_2 = -1.009606933 y_0 + 0.0310653405 y_1 = 17.23056 \]  \tag{4.31}\]

Using the RG values we find

\[d_3(RG) + 0.01950310416 d_1(RG) + 0.1410349007 d_2(RG) = 17.17371 \]  \tag{4.32}\]

in extremely close agreement (0.33% relative error) with the Padé prediction (4.31).

The insensitivity of Padé predictions of \(d_1\) for the vector correlator is to be contrasted with corresponding predictions for the scalar fermionic current correlation function considered in Section 2. If we apply the large-L asymptotic expansion of (2.7) to this scalar correlator, with \(R_1 - 3\) as given in (2.4-6), we can predict APAP\(^{\prime}\) values for \(d_4, d_3, d_2\) and \(d_1\). These values are tabulated in Table 7 alongside the APAP estimates already listed in Table 3. As is evident from the Table, both Padé methods predict quite similar values \(d_4, d_3\) and the sub-leading coefficient \(d_2\), with the asymptotic large-L expansion (APAP\(^{\prime}\)) approach showing even greater accuracy than the moment-integral (APAP) approach delineated in Section 2. For the scalar correlator, the APAP\(^{\prime}\) approach does not show signs of breaking down until the third subleading order of (2.7)’s large-L expansion, the coefficient \(d_1\), for which APAP\(^{\prime}\) is considerably less reliable than APAP. This observation is confirmed by a \(\chi^2\) minimization analysis of the scalar correlation function, which shows that the \(d_k\) are much less sensitive to any poorly determined \(y_i\).

Thus we see that different asymptotic Padé estimates do an excellent job of predicting leading and subleading \(O(x^4)\) coefficients for both the vector \((d_2, d_3)\) and the scalar \((d_3, d_4)\) fermionic current correlators. However, the approaches diverge drastically in predicting the sub-subleading term \((d_1)\) in the vector correlator, indicative of the limitations of the Padé method for this case. By contrast, the sub-subleading term \((d_2)\) in the scalar coordinator is quite well predicted using either method, suggesting greater reliability of APAP predictions in the scalar channel for subsequent subleading terms.
5. Padé-Estimates of RG-Inaccessible Coefficients

We have seen that the renormalization group equation may be utilized to determine all but one of the next-order coefficients in current correlation functions. Specifically, the coefficient $d_1$ in scalar (2.19) and vector (4.12) fermion-current correlation functions, as well as the coefficient $c_0$ in the scalar gluon-current correlation function (3.2), are not subject to RG constraints. However, knowledge of these constants is vital to a number of phenomenological applications, such as higher order perturbative contributions to QCD sum-rules, which may be large at low $s_0$ [3], or the $\mathcal{O}(\alpha_s^3)$ term in $R \equiv \sigma(e^+e^- \rightarrow \text{hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)$.

Up until now, our emphasis has been on demonstrating how asymptotic Padé-approximant methods can estimate RG-accessible coefficients within the correlators (2.17), of (3.2), and (4.12). However, it is evident from Tables 3, 4, 5 and 6 that the accuracy of such estimates diminishes as the subscript index $i$ of coefficients $d_i$ and $c_i$ decreases. The APAP predictions for $d_0$ in Table 5, for example, are quite suspect because of the insensitivity of APAP predictions to $d_0$ and $d_1$ in this channel, as discussed in the previous section.

To obviate these difficulties, we can estimate $d_0$ ($c_0$) for fermion (gluon) correlators by first averaging the asymptotic Padé-approximant expression for $R_4(w)$ [$R_3(w)$] over the interval $0 < w < 1$, and by then removing the known contributions of RG-accessible coefficients $d_{1-4}$ ($c_{1-3}$) to this average. For the scalar fermion-current correlation function, this procedure amounts to the use of RG-determined coefficients within (2.11):

$$d_0 = \int_0^1 R_4(w)dw - d_1(RGE) - 2d_2(RGE) - 6d_3(RGE) - 24d_4(RGE).$$  \(5.1\)

The integral in (5.1) is just the integral $N_{-1}$ tabulated in Table 3, where RG-values of $d_{1-4}$ are also listed. These new estimates [labelled $d_0$(APAP')] are presented in Table 8 for $n_f$ values of phenomenological interest, and are compared to the prior estimates of Table 3 obtained from higher-moment integrals. The two predictions are comparable for $n_f = 3, 4$, but quite far apart for $n_f = 6$.

Corresponding predictions for the scalar gluon-current correlation function may be obtained from rearrangement of (3.9):

$$c_0 = \int_0^1 R_3(w)dw - c_1(RGE) - 2c_2(RGE) - 6c_3(RGE),$$  \(5.2\)

with $c_{1-3}$(RG) and the integral ($P_0$) as given in Table 4. These new predictions for $c_0$, labelled as $c_0$(APAP’) in Table 9, are in good agreement with the previous Table 4 predictions $c_0$(APAP) for $n_f \leq 4$, reflecting the somewhat better agreement of Table 4’s predictions with RG values.

Finally, $d_0$ estimates for the vector fermionic correlator

$$d_0 = N_{-1} - d_1(RGE) - 2d_2(RGE) - 6d_3(RGE),$$  \(5.3\)

with all constants on the right hand side as tabulated in Table 5, are displayed in Table 10. Here the discrepancy with prior APAP estimates is quite large, but within a factor of 2 for the phenomenologically important $n_f = 5$ case. We reiterate, however that the Table 5 estimates of $d_0$ are likely skewed by the factor-of-two disparity between corresponding estimates of $d_1$ versus RG determinations of $d_1$. Consequently, we regard the top line estimates of Tables 8-10 to be the ones to be tested against future calculation.

As just one such example, the quantity $R(s)$ is obtained entirely from the nonlogarithmic coefficients within (4.12):

$$R(s) \equiv \sigma(e^+e^- \rightarrow \gamma \rightarrow \text{hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-) = 3\sum_f Q_f^2[1 + x + b_0x^2 + c_0x^3 + d_0x^4...].$$  \(5.4\)

The coefficients $b_0$ and $c_0$ are given by (4.13) in terms of constants listed in (4.2-6), and are also tabulated in Table 10. Thus, for five active flavours we predict that

$$R(s) = \frac{11}{3}[1 + x + 1.40924x^2 - 12.8046x^3 + 31.5x^4],$$  \(5.5\)

where the well-known first four terms [7,9] have been augmented by the $n_f = 5$ APAP’ estimate for $d_0$ in Table 10.
This prediction for the $x^4$ term in (5.5) differs in both sign and magnitude from an earlier Padé-motivated prediction [10]. The prediction is also substantially less than the $73.5x^4$ term one would obtain applying (2.7) directly to the first three terms in (5.5). Such an approach, however, is based on the constants $b_0$ and $c_0$ only, corresponding to finding $R_4(w)$ only for the specific choice $w = 1$ within (2.7). By contrast, the result (5.5) devolves from an estimate incorporating our exact knowledge of all coefficients $b_i$, $c_i$, and $d_i$ (except $d_0$) to find the average value of $R_4(w)$ over the full range of $w$.

In Table 10, the exact values for $b_0$ and $c_0$ are tabulated for $n_f = \{2, 3, 4\}$ as well. These values can be substituted into (5.4) to display $n_f = \{3, 4\}$ expressions for $R(s)$ which incorporate the APAP′ estimate for $d_0$. It is interesting to note that the predicted magnitude of the $x^4$ coefficients in $R(s)$ is quite modest, suggesting that the accuracy of phenomenology based on the preceding three subleading orders of perturbation theory is not compromised by higher-order corrections.

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Table 1: Coefficients of $\mathcal{O}(\alpha_s)$, $\mathcal{O}(\alpha_s^2)$ and $\mathcal{O}(\alpha_s^3)$ in terms within the fermionic scalar-current correlation function, as defined in (2.1).

| $n_f$ | $a_0$   | $a_1$ | $b_0$    | $b_1$    | $b_2$ | $c_0$ | $c_1$    | $c_2$ | $c_3$   |
|------|---------|-------|----------|----------|-------|-------|----------|-------|---------|
| 4    | $17/3$  | 2     | 30.5054  | 30.4444  | 4.08333 | 65.1980 | 267.589  | 104.384 | 8.39352 |
| 5    | $17/3$  | 2     | 29.14671 | 29.2222  | 3.91667 | 41.7576 | 238.381  | 94.6759 | 7.61574 |
| 6    | $17/3$  | 2     | 27.7881  | 28.0000  | 3.75000 | 18.8351 | 209.970  | 85.3750 | 6.87500 |

Table 2: Coefficients of QCD $\beta$- and $\gamma$-functions, as defined in (2.20) and (2.21).

| $n_f$ | $\beta_0$  | $\beta_1$  | $\beta_2$  | $\gamma_1$  | $\gamma_2$  | $\gamma_3$  |
|------|-------------|-------------|-------------|-------------|-------------|-------------|
| 0    | 11/4        | 29/12       | 9/4         | 25/12       | 7/4         |             |
| 2    | 51/8        | 115/24      | 4           | 77/24       | 13/8        |             |
| 3    | 2857/128    | 48241/3456  | 384         | 21943/3456  | 9769/128    | -65/128     |
| 4    | -           | 3.93056     | 3.79166     | 3.65277     | 3.51389     | 3.37500     |
| 5    | -           | 14.8393     | 12.4202     | 9.94702     | 7.41985     | 4.83866     |
| 6    | -           | 61.8794     | 44.2688     | 27.3088     | 11.0401     | -4.50240    |

Table 3: Comparison of asymptotic Padé-approximant predictions (APAP) to renormalization-group equation (RGE) determinations of the $\mathcal{O}(\alpha_s^4)$ coefficients $d_1 - d_4$ within the fermionic scalar-current correlation function. The integrals $N_i$, as defined by (2.8) are obtained numerically from the APAP estimate (2.10) of $R_4$, with the lower-order coefficients $a_i, b_i, c_i$ (Table 1) determining $R_{1,2,3}$. APAP estimates of $d_0 - d_4$ are obtained from these integrals via (2.11-15). RGE determinations of $d_1 - d_4$ are obtained via (2.22-25), with $\beta_i$ and $\gamma_i$ values as given in Table 2.
Table 4: The first five rows list known terms of the gluonic scalar-current correlation function (3.2). The integrals $P_{0-3}$, as defined by (3.7), are obtained numerically and utilized to obtain asymptotic Padé-approximant (APAP) estimates of the next-order coefficients $c_{0-3}$ in the gluonic correlator. Renormalization-group equation (RG) determinations of $c_1$, $c_2$, and $c_3$ are also tabulated to illustrate the accuracy of the APAP method.
Table 5: Comparison of asymptotic Padé-approximant predictions (APAP) to renormalization-group equation (RGE) determinations of the $O(\alpha_s^4)$ coefficients $d_i$ within the fermionic vector-current correlation function. The integrals $N_k$, as defined by (2.8), are obtained numerically from the APAP estimate (2.7) of $R_4$. APAP estimates of $d_0 - d_3$ are obtained from these integrals, as described in the text.

| $n_f$ | $N_{-1}$ | $N_0$ | $N_1$ | $N_2$ |
|-------|---------|-------|-------|-------|
| 2     | 160.31  | 24.56 | 11.81  | 10.17 |
| 3     | 118.82  | 20.69 | 13.94  | 14.31 |
| 4     | 86.17   | 21.18 | 19.91  | 22.37 |
| 5     | 63.94   | 26.10 | 29.59  | 34.18 |

| $d_0$(APAP) | 20.51 | 27.54 | 40.22 | 58.83 |
|----------|-------|-------|-------|-------|
| $d_1$(APAP) | -79.88 | -83.30 | -98.87 | -130.3 |
| $d_1$(RGE) | -35.49 | -46.24 | -56.90 | -63.99 |

Table 6: Padé estimates $d_1$(APAP') for the vector correlator, as obtained via large-L asymptotic expansion of (2.7), are compared to the exact results $d_1$(RG) and to the Padé estimates $d_1$(APAP) of Table 5 obtained through use of (2.7) in integrands of moment integrals $N_k$ (2.8). The two Padé estimates are seen to straddle the exact result.

| $n_f$ | $d_1$(APAP') | $d_1$(RG) | $d_1$(APAP) |
|-------|-------------|----------|-------------|
| 2     | -11.48      | -24.20   | -36.33      |
| 3     | -24.20      | -36.33   | -44.84      |
| 4     | -36.33      | -44.84   | -63.99      |
| 5     | -44.84      | -63.99   | -130.3      |
Table 7: Padé estimates $d_i(\text{APAP}')$ of coefficients $d_i$ for the fermionic scalar-current correlator, as obtained via large-$L$ asymptotic expansion of (2.7), are compared to exact (RGE) results and to the APAP estimates of Table 3. The APAP' estimates are seen to predict $d_4$, $d_3$, and $d_2$ with even better accuracy than the APAP estimates, but to suffer substantially diminished accuracy in predicting $d_1$.

| $n_f$ | $d_4(\text{APAP}')$ | $d_4(\text{RGE})$ | $d_4(\text{APAP})$ | $d_3(\text{APAP}')$ | $d_3(\text{RGE})$ | $d_3(\text{APAP})$ | $d_2(\text{APAP}')$ | $d_2(\text{RGE})$ | $d_2(\text{APAP})$ | $d_1(\text{APAP}')$ | $d_1(\text{RGE})$ | $d_1(\text{APAP})$ |
|-------|----------------------|---------------------|---------------------|----------------------|---------------------|---------------------|----------------------|---------------------|---------------------|----------------------|---------------------|---------------------|
| 3     | 20.183               | 20.143              | 20.38               | 355.5                | 356.03              | 345.7               | 1617                 | 1583.6              | 1695                | 1450                 | 1563.0              | 1339               |
| 4     | 17.323               | 17.312              | 16.63               | 305.0                | 305.73              | 307.4               | 1380                 | 1338.9              | 1398                | 244.7                | 1159.8              | 1030               |
| 5     | 14.745               | 260.06              | 15.37               | 259.2                | 1114.7              | 1177                | 1111                 | 1114.7              | 1177                | 2582                 | 791.52              | 744.9               |
| 6     | 12.434               | 218.82              | 17.29               | 217.9                | 910.31              | 1067                | 916.2                | 910.31              | 405.6               | 457.39               | 442.2               |                     |

Table 8: Asymptotic Padé-approximant predictions of the $d_0$-coefficient in the scalar fermion-current correlation function. $d_0(\text{APAP}')$ is obtained from (5.1) using renormalization-group determinations of $d_1-4$, as given in Table 3. $d_0(\text{APAP})$ are previous predictions obtained in Table 3 without RG-inputs.

| $n_f$ | $d_0(\text{APAP}')$ | $d_0(\text{APAP})$ |
|-------|---------------------|---------------------|
| 3     | 195                 | 252                 |
| 4     | 130                 | 147                 |
| 5     | 115                 | 64.2                |
| 6     | 156                 | 9.00                |

Table 9: Asymptotic Padé-approximant predictions of the $c_0$-coefficient in the scalar gluon-current correlation function. $c_0(\text{APAP}')$ is obtained from (5.2) using renormalization-group determinations of $c_1-3$, as given in Table 4. $c_0(\text{APAP})$ are previous predictions obtained in Table 4 without RG-inputs.

| $n_f$ | $c_0(\text{APAP}')$ | $c_0(\text{APAP})$ |
|-------|---------------------|---------------------|
| 0     | 4022                | 4262                |
| 2     | 2179                | 2345                |
| 3     | 1442                | 1580                |
| 4     | 834.3               | 950.4               |
| 5     | 366.4               | 466.0               |
| 6     | 55.6                | 144.5               |

Table 10: Asymptotic Padé-approximant predictions of the $d_0$-coefficient in the vector fermion-current correlation function. $d_0(\text{APAP}')$ is obtained from (5.3) using renormalization-group determinations of $d_1-3$, as given in Table 5. $d_0(\text{APAP})$ are previous predictions obtained in Table 5 without RG-inputs. Exact values of $b_0$ and $c_0$ [7,9] are also displayed to facilitate use of (5.4) to obtain $n_f = 3, 4$ expressions for $R(s)$.

| $n_f$ | $d_0(\text{APAP}')$ | $d_0(\text{APAP})$ | $c_0$ | $b_0$ | $d_0$ |
|-------|---------------------|---------------------|-------|-------|-------|
| 2     | -8.29               | 20.5                | -9.14051 | 1.75512 | 31.5  |
| 3     | 1.90                | 27.5                | -10.2839 | 1.63982 | 15.7  |
| 4     | 15.7                | 40.2                | -11.6856 | 1.52453 | 15.7  |
| 5     | 31.5                | 58.8                | -12.8046 | 1.40924 | 31.5  |
| 6     |                    |                     |       |       |       |