Comparison of the Padé Approximation Method to Perturbative QCD Calculations

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We present a method of estimating perturbative coefficients in quantum field theory using Padé approximants. We test this method on various known quantum chromodynamics (QCD) results, and find that the method works very well.

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By using the first \( n \) coefficients in a series expansion, we have estimated the \((n + 1)\text{st}\) perturbative coefficient in quantum field theory (QFT). Though there is currently no theoretical basis for extrapolating coefficients in the perturbative loop expansion of QFT by our method, our results have thus far been in good agreement with the calculated coefficients of quantum electrodynamics (QED), as well as with series in statistical physics, condensed matter theory, and mathematics [1–6]. In this Letter we compare our method to the perturbative loop expansion of quantum chromodynamics (QCD) at the five-loop level. We shall present results for the \( R \) ratio, the \( R_f \) ratio, the QCD \( \beta \) function, and two QCD sum rules.

Our method makes use of Padé approximants (PA) and enables us to obtain an estimate and an error bar for each coefficient. We define the PA

\[
[N/M] = \frac{a_0 + a_1X + \cdots + a_NX^N}{1 + b_1X + \cdots + b_MX^M}
\]

(1)
to the series \( S \) where we set

\[
[N/M] = S + O(X^{N+M+1}) \quad \text{and} \quad S = \sum_{n=0}^{\infty} S_nX^n.
\]

(2)

One solves Eq. (2) and then predicts the coefficient of the next term \( S_{N+M+1} \). This is what we do in this Letter. One can also use the full PA to estimate the sum of the whole series \( S \). This is what we will do in the future [7,8]. For a detailed description, see Refs. [5] and [6].

The PA’s are known to accelerate the convergence of many series by including the effects of higher (unknown) terms, thus providing a more accurate estimate of the series. We have recently proved the following theorem, which provides a useful sufficient condition for the PA’s to be accurate. Defining \( f(n) = \ln S_n \) and considering

\[
g(n) = \frac{d^2f(n)}{dn^2},
\]

(3)
a sufficient condition for the PA’s to converge is that

\[
lm(n) = 0.
\]

(4)
The PA’s thus provide reliable estimates of asymptotic series whose coefficients diverge as

\[
S_n = n!k^n\gamma^n,
\]

(5)
as is believed to be the case in QED and QCD [9]. It can easily be shown that Eq. (4) is satisfied for \( S_n \) given by Eq. (5). In the cases of these and other series whose Borel transform has a finite radius of convergence, the higher-order PA’s give progressively better approximations to the principal value of the transform integral over Borel singularities. It is easy to check that for series with one or two simple Borel poles (i.e., IR and UV renormalons); Padé approximants predict the next term in a given series with a rapidly increasing precision. In these cases an analytic estimate \( -M!N^M \) can be made for the relative error of the \([N/M]\) Padé approximant prediction of the next term in the series.

It might be objected, however, that these cases are not sufficiently complicated to be realistic. Therefore, as an exercise, we have evaluated Padé approximants to the large-\( N_f \) limit of the vacuum polarization \( D \) function in QCD, which is known to all orders in \( \alpha_s \), and whose Borel transform contains an infinite series of double poles at both positive and negative integers [10]. Once again, as seen in Fig. 1, the Padé approximants’ predictions of the next term in the series converge rapidly, in agreement with the above-mentioned estimated error for the \([N/M]\) Padé approximant. The convergence of the Borel transform of the \( D \)-function series, in particular, indicates that our PA approach is well suited for perturbation series with the asymptotic behavior expected in QCD.

We now turn to some QCD applications of our PA approach. Let us first consider the \( R_f \) ratio [11] where \( R_f \) is defined as follows:

\[
R_f = \frac{\Gamma(\tau \to \nu + \text{hadrons})/\Gamma(\tau \to e\nu \bar{\nu})}{3S_{\text{EW}}(r_f + r_f^1)}
\]

(6)
where $S_{\text{EW}} = 1.019$ is the electroweak correction and $r^1_r = -1.58\%$ is the nonperturbative contribution. The perturbative QCD contribution is given by

$$
R = 3 \sum \Omega_i^2 r_i \quad r_i = 1 + \left( \frac{\alpha_s}{\pi} \right) + 1.409 \left( \frac{\alpha_s}{\pi} \right)^2 - 12.805 \left( \frac{\alpha_s}{\pi} \right)^3 - (87.5 \pm 10.8) \left( \frac{\alpha_s}{\pi} \right)^4.
$$

(10)

The last term in Eq. (10) is our estimate for the five-loop contribution to $R$ where we here extrapolated the related Adler $D$ function. Using Eq. (9) we obtain

$$
r(34 \text{ GeV}) = 1 + 0.0445 + 0.0028 - 0.0011 - 0.0003 = 1.0459(4).
$$

(11)

This series for $r$ is Eq. (11), where the contributions in each order, up to five loops, are given, seems to converge nicely. Experimentally there are two measurements of $r(34 \text{ GeV})$. They are $r(34 \text{ GeV}) = 1.049(7)$ [15] and $r(34 \text{ GeV}) = 1.056(8)$ [16]. It can be seen that the extrapolation prediction in Eq. (11) is in good agreement with these experimental values. We can now evolve $\alpha_s$ up to $M_Z$, the $Z$ boson mass. Our result

$$\alpha_s(M_Z) = 0.119(2),$$

(12)

which is consistent with the latest experimental value obtained from total-cross-section measurements at the CERN $e^+e^-$ collider LEP [17]

$$\alpha_s(M_Z) = 0.126(6).$$

(13)

For $r$ at $M_Z$ we get $r(M_Z) = 1 + 0.0378 + 0.0020 - 0.0007 - 0.0002 = 1.0389(2)$.

We now present our estimates for higher-order perturbative coefficients for $R$, $R_r$, the QCD $B$ function, and two QCD sum rules. All of the results presented here are in the MS scheme. The corresponding results for other schemes can also be obtained. However, the scheme dependence should decrease in higher order, disappearing if all orders are known.

To provide systematic-error estimates, we first apply our method to $S_n$, obtaining our estimate $S^{(0)}_{n+1}$. We then apply it to the reciprocals $r_n = 1/S_n$, and take the reciprocal again to obtain $S^{(1)}_{n+1}$. We then take differences $t_n = r^{(1)}_{n+1} - r_n$ and apply our method to obtain a third estimate $S^{(2)}_{n+1}$. Our systematic-error estimate is $\Delta / 2$, where $\Delta = |S^{(2)}_{n+1} - S^{(1)}_{n+1}|$. We then combine the diagonal and nondiagonal estimates of $S_{n+1}$, weighted by $1/\Delta$, to obtain our final estimate for $S_{n+1}$.

In Table I we present our results for $R$ and $R_r$. The first entry in each case is the four-loop result. The light-by-light contribution is small but should be added to $R(\text{MS})$. Our estimates of the four-loop coefficients, based on PA's to lower-order coefficients, agree well with the known exact results, providing a sound phenomenological footing for our method. The second entries are our estimates

$$
\alpha_s(34 \text{ GeV}) = 0.1399(11).
$$

(9)

For the $R$ ratio, we have [14]
for the five-loop coefficients, and the numbers in brackets are our estimate of the systematic errors. The results $-96.8$ (KS) and $105.5$ (KS) are the estimates of Ref. [18], obtained using a completely independent method, optimized perturbation theory (OPT). The agreement with our estimates is very good.

In Table II we present our results for the QCD $\beta$ function. The agreement with the known three-loop results is very good, and we present the first estimates of the four-loop QCD $\beta$ function. Note that the three- and four-loop results are scheme dependent, and we use the MS scheme throughout. The three-loop result is the same for any MS-type scheme. Since we use the MS result for the three-loop coefficient, our estimate for the four-loop coefficient is also for the MS scheme.

In Table III we present our results for the Bjorken sum rule for deep inelastic (unpolarized) neutrino-nucleon scattering. To compare with Ref. [18], we multiply their results by $-2/3$. Our results for $O(\alpha_s^3)$ are very good again, and again the agreement with Ref. [18] in $O(\alpha_s^4)$ is excellent. We present our results for the Bjorken sum rule for deep inelastic polarized electron-nucleon scattering ($-\text{BjPSR}$) in Table IV. Again our results in $O(\alpha_s^3)$ are good and our $O(\alpha_s^4)$ estimates agree with Ref. [18]. The Gross–Llewellyn-Smith sum rule (GLSSR) differs from the BjPSR by the light-by-light contribution: GLSSR = BjPSR $- 0.413 f$. The light-by-light contribution here and for $R$ should be treated separately. This contribution is small, however, for all cases of interest.

In Table V we present our results for the $R$ ratio for various $N_f$. The small difference for $N_f = 5$ compared with Table I is due to a slight difference in averaging the various estimates. The results for the four-loop coefficients are excellent, and the agreement with Ref. [18] for the five-loop coefficients is satisfying.

Although it is interesting that our estimates for the next term agree with Ref. [18] and we believe both of us are right, we cannot be certain. Both of us may be wrong. Fortunately, even a crude estimate of the next term is sufficient since their contributions to the full series are small. However, it is important to know they are small.

In conclusion, we have used our estimation method, which makes use of Padé approximants, to estimate various perturbative coefficients in QCD. Our estimates for the known terms are very good. Moreover, our estimates for the next unknown terms agree very well with the results of Ref. [18] in all cases where comparison is possible.

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<tr>
<th>Series</th>
<th>Estimate</th>
<th>Exact</th>
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<tbody>
<tr>
<td>N_f = 3</td>
<td>-455(228)</td>
<td>-644</td>
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<tr>
<td></td>
<td>-5920(1956)</td>
<td></td>
</tr>
<tr>
<td>N_f = 4</td>
<td>-316(158)</td>
<td>-406</td>
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<tr>
<td></td>
<td>-3058(875)</td>
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<tr>
<td>N_f = 5</td>
<td>-195(49)</td>
<td>-181</td>
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<tr>
<td></td>
<td>-845(105)</td>
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<table>
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<tr>
<th>Series</th>
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<tr>
<td>N_f = 3</td>
<td>-12.8(6.4)</td>
<td>-20.2</td>
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<td></td>
<td>-112(33)</td>
<td>-130 (KS)</td>
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<td>N_f = 4</td>
<td>-10.6(4.4)</td>
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<td></td>
<td>-58.2(15.2)</td>
<td>-68.1 (KS)</td>
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<td>N_f = 5</td>
<td>-8.5(3.4)</td>
<td>-7.8</td>
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<tr>
<td></td>
<td>-21.1(3.4)</td>
<td>-17.8 (KS)</td>
</tr>
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</table>
TABLE V. Estimates for $R(MS)$ for various $N_f$ at the four-
(first row) and five-loop (second row) order. The four-loop
results are compared with the exact (known) results, and the
five-loop results are compared with those of KS.

<table>
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<tr>
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<th>Estimate</th>
<th>Exact</th>
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<tr>
<td>$N_f = 3$</td>
<td>$-14.1 \pm 2.0$</td>
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<td>$-119.3 \pm 6.3$</td>
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<td>$-115.2 \pm 5.4$</td>
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<td>$N_f = 5$</td>
<td>$-10.07 \pm 1.99$</td>
<td>$-12.76$</td>
</tr>
<tr>
<td></td>
<td>$-86.5 \pm 10.8$</td>
<td>$-96.8$ (KS)</td>
</tr>
</tbody>
</table>

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Note added.—A phenomenological extraction of the
five-loop $D$-function coefficient from measured moments
of $\tau$ decay data has recently appeared [19], which
confirms our prediction. In the process of our analysis
we are comparing our results with explicit expressions
given in Ref. [14] and in papers listed in Ref. [18]. The
original references for the NNLO calculations are as
follows: $R(s)$ [14,20]; the QCD beta function [21]; the
Bjorken nonpolarized sum rule [22]; and the Bjorken
polarized sum rule [23]. We thank Andrei Kataev for
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    and M. A. Samuel (World Scientific, Singapore, 1991); L. R. Surguladze and M. A. Samuel, Phys. Rev. Lett. 66,

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4383