Estimating higher order perturbative coefficients using Borel transform

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Abstract

A new method of estimating higher order perturbative coefficients is discussed. It exploits the rapid, asymptotic growth of perturbative coefficients and the information on the singularities in the complex Borel plane. A comparison with other methods is made in several Quantum Chromodynamics (QCD) expansions.

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The ordinary perturbative expansions in weak coupling constant in quantum field theories are generally asymptotic expansions, with their perturbative coefficients growing factorially at large orders [1]. In practice, in many cases the asymptotic growth sets in quite early in perturbation, and the rapid growth of the coefficients becomes apparent already at first few orders.

The asymptotic divergence of the perturbative coefficients implies singularities in the Borel plane. There are three kinds of known singularities, all on the real axis: those instanton-induced, ultraviolet renormalons, and infrared renormalons.

In this paper, we show that this rapid growth of the perturbative coefficients and the information on the singularities in the Borel plane can be turned into a useful tool that allows us to estimate the unknown \((N + 1)\)th order coefficient using the known coefficients up to order \(N\). The method we are going to present can be most easily understood by working out an explicit example, the double-well potential in quantum mechanics. The tunneling between the two potential wells splits the degenerate perturbative ground states into a parity even, and an odd states, and the average energy \(E(\alpha)\) of the energies of these two states has the perturbative expansion of the form

\[
E(\alpha) = - \left[ \alpha + \sum_{n=1}^{\infty} a_n \alpha^{n+1} \right],
\]

where \(\alpha\) denotes the canonical coupling of the model [2]. The Borel transform \(\tilde{E}(b)\) of \(E(\alpha)\), which has the perturbative expansion

\[
\tilde{E}(b) = - \left[ 1 + \sum_{n=1}^{\infty} a_n b^n \right],
\]

is known to have multi-instanton–anti-instanton caused singularities at \(b = 2nS_0\), \((n = 1, 2, 3, \cdots)\), where \(S_0 = 1/6\) is the one-instanton action (in units of \(1/\alpha\)).

The nature of the singularities can in principle be determined by doing perturbation in the background of multi-instanton–anti-instanton configurations. The closest singularity to the origin at \(b = 1/3\), which determines the leading large order behavior of the expansion (1), can be shown to have the following form [3]

\[
\tilde{E}(b) = \frac{9}{\pi(1-3b)^2} \left[ 1 - \frac{53}{18}(1-3b) + O[(1-3b)^2 \ln(1-3b)] \right] + \text{Analytic part},
\]

which comes from the instanton–anti-instanton contributions to \(E(\alpha)\). The “Analytic part” denotes terms that are analytic around the singularity.

We now consider the function \(R(b) \equiv (1-3b)^2 \tilde{E}(b)\) as introduced in [4], to control the divergence at the singularity. \(R(b)\) is bounded at \(b = 1/3\), and has a very soft singularity, a suppressed logarithmic cut. Thus the power expansion of \(R(b)\) around the origin is expected to better behave than that of \(\tilde{E}(b)\). Ignoring the residual logarithmic cut, we would expect the convergence radius of the former is bounded by the second singularity at \(b = 2/3\), thus effectively to become twice that of the latter. To make the expansion of \(R(b)\) better, we can take a further step of conformally mapping the singularities except the first one as far away as possible from the origin. This way one can hope to have a smoother \(R\) in the new plane, and a better behavior of the expansion.
Double well-potential

|    | $a_1$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ |
|----|------|------|------|------|------|
| Exact | 4.5  | 44.50 | 626.625 | 1.103 $10^4$ | 2.288 $10^5$ |
| Est. | 6.0  | 33.75 | 600.047 | 1.070 $10^4$ | 2.266 $10^5$ |

TABLE I. The exact and the estimated coefficients of the vacuum energy of the double-well potential.

The conformal mappings we consider in this paper are such that all the singularities in the Borel plane except the first one are mapped to the unit circle and the first one to a point within the circle [5]. Such a mapping in this case is given by

$$w = \frac{1 - \sqrt{1 - 3b/2}}{1 + \sqrt{1 - 3b/2}}$$  (4)

which maps the first singularity to $w_0 = (\sqrt{2} - 1)/(\sqrt{2} + 1) = 0.171$ and all others to the unit circle. Without the residual cut-singularity, $R$ would be analytic on the unit disc in the $w$-plane.

Now the power expansion of $R(b(w))$ up to $O(w^5)$ is

$$R = 1 + \sum_{n=1}^{\infty} r_n w^n$$

$$= 1 + (-16 + 2.667 a_1)w + (-120 + 3.556 a_2)w^2 + (-1896.44 + 3.161 a_3)w^3 +$$

$$(-22544 + 2.107 a_4)w^4 + (-254667.7 + 1.124 a_5)w^5 + \cdots$$

$$= 1 - 4w + 38.22w^2 + 84w^3 + 699.1w^4 + 2538.1w^5 + \cdots$$  (6)

where the coefficient at a given order in (5) was calculated using the exact values of $a_n$, which are given in Ref. [2], up to that order less one, and the coefficients in (6) were obtained with the exact values of $a_n$. What is interesting about this expansion is that the $a_n$-independent constant term in the coefficient at a given order in (5) is much larger than the exact value of the corresponding $r_n$ in (6). This then implies that a good approximate estimate of $a_n$ can be obtained by simply putting

$$r_n = 0$$  (7)

in (5). The estimated values for $a_n$ from this prescription are given in Table I, which shows improving accuracy as the order grows, and the accuracy becomes better than 1% at $n = 5$.

Obviously, the success of this method relies on the exact value of $r_n$ being much smaller than the constant term in the corresponding coefficient in expansion (5). We may understand this feature in the following way. We note first the coefficient $r_n$ is a linear combination of $a_i$’s ($i \leq n$), which are large numbers. For the sake of argument, let us ignore for the moment the soft cut-singularity of $R$ at $w = w_0$. Then $R$ is analytic on the unit disk in $w$-plane, and so we expect the growth of $r_n$ is fundamentally limited. To yield a small number out of large numbers, this then suggests a delicate cancellation occur among the large numbers in the expression for $r_n$. However, when $r_n$’s are written as in expansion (5), the cancellations
are incomplete, yielding the large constant terms. This account shows that the essential ingredients for the success of our prescription are: (i) rapid growth of the perturbative coefficients, and (ii) information on the nature and locations of the Borel plane singularities. One may notice the exact values of \( r_n \)'s in (6) still grow quite rapidly. This may be due to the residual logarithmic cut, and the infinite number of singularities on the unit circle.

With this example in mind, we now give the general prescription for estimating uncalculated higher order coefficients. Let us suppose an amplitude \( A(\alpha) \) and its Borel transform in a given theory have the perturbative expansion of the form

\[
A(\alpha) = \alpha + \sum_{n=1}^{\infty} a_n \alpha^{n+1}
\]

(8)

with \( \alpha \) denoting the canonical coupling of the theory, and

\[
\tilde{A}(b) = 1 + \sum_{n=1}^{\infty} a_n \frac{b^n}{n!}
\]

(9)

The overall normalization of the expansion (8) was chosen such that the coefficient of the leading term is unit. We assume the Borel transform \( \tilde{A}(b) \) has singularities on the real axis on the \( b \)-plane, and the first two singularities on the positive real axis are at \( b = b_0 \), and at \( b = b_1 \), respectively, and the first singularity on the negative real axis is at \( b = -b_{-0} \). We further assume the nature of the first singularity on the positive real axis is known, and is of the form

\[
\tilde{A}(b) = \frac{C}{(1-b/b_0)^{1+\nu}}[1 + O(1-b/b_0)] + \text{Analytic part},
\]

(10)

with \( C \) a real constant and the ‘Analytic part’ denoting terms analytic about \( b = b_0 \). We now introduce a conformal mapping

\[
w = \sqrt{\frac{1+b/b_{-0} - \sqrt{1-b/b_1}}{1+b/b_{-0} + \sqrt{1-b/b_1}}},
\]

(11)

which maps the first singularity on the positive axis to a point within the unit circle and all others to the circle, and the function

\[
R(b) = (1-b/b_0)^{1+\nu} \tilde{A}(b).
\]

(12)

We then expand \( R(b(w)) \) in power series in \( w \)-plane:

\[
R = 1 + \sum_{n=1}^{\infty} r_n w^n
\]

\[
= 1 + \sum_{n=1}^{\infty} (p_n + q_n a_n) w^n.
\]

(13)

Note that \( p_n, q_n \) depend linearly on the leading coefficients to \( a_n \) only. The estimated \( n \)th order coefficient is then given by
**Bjorken polarized sum rule**

| \(N_f\) | \(d_1^{\text{ext.}}\) | \(d_1^{\text{est.}}\) | \(d_2^{\text{ext.}}\) | \(d_2^{\text{est.}}\) | \(d_2^{\text{PMS}}\) | \(d_2^{\text{ECH}}\) | \(d_3^{\text{est.}}\) | \(d_3^{\text{PMS}}\) | \(d_4^{\text{est.}}\) | \(d_4^{\text{PMS}}\) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.25 | 3.86 | 34.01 | 27.36 | 28.41 | 27.25 | 302 | 290 | 3750 | 2716 |
| 2 | 3.92 | 3.51 | 26.94 | 23.17 | 24.09 | 23.11 | 223 | 203 | 2515 | 1696 |
| 3 | 3.58 | 3.14 | 20.22 | 19.21 | 20.01 | 19.22 | 156 | 130 | 1565 | 933 |
| 4 | 3.25 | 2.73 | 13.85 | 15.46 | 16.16 | 15.57 | 101 | 68 | 867 | 396 |
| 5 | 2.92 | 2.29 | 7.84 | 11.90 | 12.59 | 12.19 | 60 | 18 | 388 | 56 |
| 6 | 2.58 | 1.79 | 2.19 | 8.48 | 9.29 | 9.08 | 31 | -22 | 95 | -115 |

**Adler function**

| \(N_f\) | \(d_1^{\text{ext.}}\) | \(d_1^{\text{est.}}\) | \(d_2^{\text{ext.}}\) | \(d_2^{\text{est.}}\) | \(d_2^{\text{PMS}}\) | \(d_2^{\text{ECH}}\) | \(d_3^{\text{est.}}\) | \(d_3^{\text{PMS}}\) | \(d_4^{\text{est.}}\) | \(d_4^{\text{PMS}}\) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.87 | 3.45 | 14.11 | 8.18 | 8.71 | 7.54 | 66 | 75 | 693 | 550 |
| 2 | 1.76 | 3.19 | 10.16 | 7.19 | 7.55 | 6.57 | 43 | 50 | 391 | 316 |
| 3 | 1.64 | 2.90 | 6.37 | 6.26 | 6.40 | 5.61 | 24.4 | 27.5 | 165 | 151 |
| 4 | 1.53 | 2.58 | 2.76 | 5.37 | 5.27 | 4.68 | 9.9 | 8.4 | 8.04 | 49 |
| 5 | 1.41 | 2.22 | -0.69 | 4.50 | 4.16 | 3.77 | 0.35 | -7.7 | -87 | 2.47 |
| 6 | 1.30 | 1.80 | -3.96 | 3.59 | 3.08 | 2.88 | -3.48 | -21 | -129 | 4.18 |

**TABLE II.** The Bjorken polarized sum rule and the Adler function: Estimated values along with the exact values and the PMS, ECH values when available.

\[ a_n = -\frac{p_n}{q_n} \]  
\[ \delta_n = \frac{r_n}{p_n} \]

The fractional error of this estimate is

and this scheme would work as long as \( r_n \) is much smaller than \( p_n \). Of course, it is impossible to know the error \( a \text{ priori} \), and the reliability of the estimated coefficients should be decided by other circumstantial informations, for instance, as in the following examples, by the pattern of the known terms in expansion (13), or by comparison with the estimated values from using different methods. Since the expansion (13) is in general not convergent on the whole unit disc due to the residual soft singularity, and because of the singularities on the boundary of the disc, it is possible in principle for \( r_n \) at a certain order to jump to a large value. In such a case the scheme could fail, but that does not seem to occur, at least, at the orders considered in the following QCD expansions.

We now apply our scheme to the various QCD expansions, estimating the uncalculated next higher order coefficients, and compare the obtained values with the estimates from other methods. Of course, the coefficients are renormalization scheme and scale dependent, but for simplicity, in all of the following examples our consideration will be in the \( \overline{\text{MS}} \) scheme and at the renormalization scale \( \mu = Q \), where \( Q \) denotes the energy scale of the problem in consideration. The canonical coupling in these examples is \( a(Q) \equiv \alpha_s(Q)/\pi \), where \( \alpha_s(Q) \) is the strong coupling constant.

**The Bjorken sum rule:** Our first example is the QCD correction \( \Delta \) for the Bjorken polarized sum rule, which has the perturbative expansion
\[ \Delta(a) = a + \sum_{n=1}^{\infty} d_n a^{n+1}. \] (16)

Incidently, this correction coincides with that of Gross-Lewellyn Smith (GLS) sum rule at next-leading order, and differs only by the small ‘light-by-light’ contribution at next-next-leading order. The first two coefficients \( d_1, d_2 \) are known \([6]\). The locations of the first singularities of the Borel transform \( \Delta(b) \) and the parameter \( \nu \) are given as \([7]\)

\[ b_0 = \frac{1}{\beta_0}, \quad b_1 = \frac{2}{\beta_0}, \quad b_{-0} = \frac{1}{\beta_0}, \quad \nu = (\beta_1 / \beta_0 - \gamma_0) / \beta_0, \] (17)

where \( \beta_0, \beta_1 \) are the first two coefficients of the QCD \( \beta \)-function:

\[ \beta_0 = (11 - 2/3N_f)/4, \quad \beta_1 = (102 - 38N_f/3)/16, \] (18)

and \( \gamma_0 \) is the one-loop anomalous dimension of the twist-four operator appearing in operator product expansion of the sum rule \([8]\):

\[ \gamma_0 = (N_c - 1/N_c)/3 = 8/9. \] (19)

Here \( N_f, N_c \) denote the number of quark flavors and colors, respectively. These are all we need to estimate the unknown next higher order coefficients.

The result is given in Table II, alongside of the estimates from the principle of minimal sensitivity (PMS) method (and the effective charge (ECH) method) by Kataev and Starshenko \([9]\). The latter is based on the optimization of the perturbative amplitude over the parameter space of the renormalization scheme and scale dependence. It estimates the uncalculated higher order coefficients by reexpanding the optimized amplitude in terms of the coupling in the particular scheme and scale of interest. The recent, exact, partial calculation of the next-next-next-leading order correction \([10]\) indicates this method, among others \([11]\), works particularly well.

The estimates from the two methods are in good qualitative agreement, with some exceptions at \( d_3 \). It is remarkable that these two completely different approaches offer such close estimates. As in PMS case, our method works best at \( N_f = 3 \), and the estimates become worse as \( N_f \) increases. Although the two approaches are in an overall agreement, the differences at \( d_3 \) estimates are large enough to be phenomenologically significant. For instance, the new estimate \( d_3 \approx 156 \) at \( N_f = 3 \), which was used in the recent GLS sum rule analysis \([12]\), results in a less renormalization scale dependent amplitude than with the PMS estimate \( d_3 \approx 130 \). It is instructive to see this estimate more closely. The expansion of \( R \), following \((13)\), at \( N_f = 3 \), reads

\[
R = 1 + \sum_{n=1}^{\infty} r_n w^n = 1 + \sum_{n=1}^{\infty} (p_n + q_n d_n) w^n
= 1 + (-3.72 + 1.185d_1)w + (-13.488 + 0.702d_2)w^2 + (-43.257 + 0.277d_3)w^3 + \cdots
= 1 + 0.527w + 0.709w^2 + \cdots
\] (20)  

where the last two terms in \((21)\) are exact. Notice that the first two \( p_n \)'s are large compared to the corresponding \( r_n \)'s, satisfying one of the absolutely necessary conditions for our scheme,
and the pattern of the first two known coefficients suggests that \( p_3 \) is also likely to be much larger than \( r_3 \). If we believe that the first two \( r_n \)'s have any indication on \( r_3 \), it seems to be safe to assume \( |r_3| \leq 2.0 \). This then leads to \( 149 \leq d_3 \leq 163 \).

The estimates of the next higher order coefficients \( d_4 \)'s are obtained using the \( d_3 \) estimates. Compared to the PMS estimates there is some significant difference at this order. Since the obtained values depend on the estimated \( d_3 \), one should note that there is another uncertainty arising from the error in \( d_3 \) estimate.

**The Adler function:** The Adler function \( D(a) \) for the vector current-current correlation function of different quark flavors has the perturbative expansion

\[
D(a) = a + \sum_{n=1}^{\infty} d_n a^{n+1}
\]

where the first two coefficients are known [13]. Several physical observables can be related to this function through the dispersion relations, and the perturbative coefficients of the former can be obtained once the corresponding coefficients in the Adler function are known.

The locations of the first renormalon singularities and \( \nu \) in this case are given by [14]

\[
b_0 = \frac{2}{\beta_0}, \quad b_1 = \frac{3}{\beta_0}, \quad b_{-0} = \frac{1}{\beta_0}, \quad \nu = 2\beta_1/\beta_0^2, \quad (23)
\]

and the resulting estimates for the first coefficients are given in Table II, along with the PMS, ECH values. Again, our method works best at \( N_f = 3 \) for the first two coefficients, and in this case the predicted \( d_3 = 24.4 \) is slightly smaller than the PMS value \( d_3 = 27.5 \).

**The quark mass:** This last example is concerned with the on-shell quark mass. The on-shell quark mass and the \( \overline{\text{MS}} \) mass are related by

\[
\frac{m_{\text{OS}}}{m_{\text{MS}}} = 1 + \frac{4}{3} \left[ a + \sum_{n=1}^{\infty} r_n a^{n+1} \right],
\]

and the first two coefficients are known [15]. The relevant parameters in this case are [16]

\[
b_0 = \frac{1}{2\beta_0}, \quad b_1 = \frac{3}{2\beta_0}, \quad b_{-0} = \frac{1}{\beta_0}, \quad \nu = \beta_1/2\beta_0^2, \quad (25)
\]
and the estimated first coefficients are in Table III, along with the values from the residue based method of Pineda [17] (also, for comparison, those of large $\beta_0$ approximation [18]), which is known to work well in this case. The latter method relies on the rapid convergence of the perturbative calculation of the renormalon residue, and the expansion of the Borel transform about the first renormalon [4,5]. The agreement between these two approaches at $r_3$ estimates is remarkable.

To conclude the paper, we presented a new method of estimating higher order unknown coefficients. It is based on the two generic features of the asymptotic expansions, the rapid growth of the coefficients and the Borel plane singularities. It can provide independent estimates for the yet unknown coefficients, which may prove useful in physical analysis.

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Postscript: After submission of our paper we were informed that in the published version [19] of hep-ph/9811367 Borel transform with a conformal mapping was tried on a model function to estimate higher order coefficients. Unlike our method, however, it did not remove the first Borel singularity, and because of that it reached to a conclusion substantially different from ours, that the method can work only for large orders (say, $N \sim 7$) and is not applicable for low orders ($N \sim 3$) relevant for present QCD perturbations.
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