Pade Approximants and Borel Summation for QCD Perturbation Expansions

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Abstract

We study the applicability of Pade Approximants (PA) to estimate a "sum" of asymptotic series of the type appearing in QCD. We indicate that one should not expect PA to converge for positive values of the coupling constant and propose to use PA for the Borel transform of the series. If the latter has poles on the positive semiaxis, the Borel integral does not exist, but we point out that the Cauchy principal value integral can exist and that it represents one of the possible "sums" of the original series, the one that is real on the positive semiaxis. We mention how this method works for Bjorken sum rule, and study in detail its application to series appearing for the running coupling constant for the Richardson static QCD potential. We also indicate that the same method should work if the Borel transform has branchpoints on the positive semiaxis and support this claim by a simple numerical experiment.

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1 Introduction

Perturbative expansions appearing in QCD and many of its models simulating various interesting features of this theory have, usually, coefficients growing so fast that it is difficult to obtain an increased precision by naive adding of subsequent terms [1], [2].

Pade Approximants (PA) are an effective tool to "sum" an asymptotic series [3], [4], however they may not necessarily sum it to the function that has the required analytic properties. We must remember that there is an infinite number of analytic functions having the same asymptotic expansion, and the additional requirements stemming from the physical meaning of the function can help us to diminish this abundance.

We shall first illustrate this problem on the very simple example and show that the use of the Borel integral can be of help here. As we expect the perturbation series in QCD to have coefficients growing like $n! K^n n^\gamma$ [2] let us consider the simplest series of this type - the Euler series:

$$e(z) = \sum_{n=0}^\infty n! z^n$$  \hspace{1cm} (1)

It is well known [3], [4] that PA to this series converge to the function:

$$E(z) = \int_0^\infty \frac{e^{-u}}{1 - zu} du$$  \hspace{1cm} (2)

in the whole complex plane with the positive semiaxis excluded. The function has the branch point at $z = 0$ and PA reconstruct the branch of this function which is real on the negative semiaxis and has cut along the positive one. In QCD the expansion parameter is usually the coupling constant and we want to have our function for the positive values of coupling constant - moreover we want, for real expansion coefficients, the function to be real, at least close to zero. Our aim is therefore to find a function which has not only the expansion (1) but is also real on the positive semiaxis. We want to stress that such function is again not unique, but we want to show how one of such functions can be constructed from (1).

We first consider a case when the Borel transform of the series has only poles (Section 2) and illustrate our point in Section 3 by two examples of QCD related series. Then, in Section 4, we apply our considerations to the case when the Borel transform has branchpoints and claim that the same approach (taking the Principal Value of the Borel integral over Pade Approximants to the Borel transform of the series) would work here - we support this claim by a simple numerical example.
2 Poles in the Borel transform

We consider the series:

\[ f(z) = \sum_{n=0}^{\infty} f_n z^n \]  

where we expect that asymptotically (for \( n \to \infty \)) \( f_n \) behaves like \( n!K^n n^\gamma \). The Borel transform of this series is then:

\[ g(z) = \sum_{n=0}^{\infty} g_n z^n = \sum_{n=0}^{\infty} \frac{f_n}{n!} z^n \]

If all \( f_n \)'s are positive (which is often the case in QCD), then we can expect that \( g(z) \) has a singularity at \( z = K \) (where \( K \) is the radius of convergence of (4)). In this case the Borel integral:

\[ \Phi(z) = \int_{0}^{\infty} e^{-u} g(uz) du \]

is complex for \( z > 0 \), if it exists. If \( g(z)(z - K) \) is finite for \( z \to K \), then this singularity does not spoil the convergence of (5), and similar conditions can be imposed on the behaviour of \( g(z) \) near other singularities.

Let us first assume that \( g(z) \) has a simple pole at \( z = K \). In this case:

\[ \lim_{z \to K} g(z)(z - K) = \text{Res}_{z=K} g(z) < \infty \]  

and the integral (5) can be written, for \( x \in (0, \infty) \) as:

\[ \Phi(x) = PV \int_{0}^{\infty} e^{-ux} g(ux) du \pm \frac{i\pi}{x} e^{-K/x} \text{Res}_{x=K} g(x) \]

- choice of the sign depends on whether in (5) we integrate just below or just above the positive semiaxis. We see that the imaginary part of \( \Phi(z) \) has all coefficients of the power expansion at \( z = 0^+ \) vanishing and therefore:

\[ \mathcal{E}(x) = Re\Phi(x) = PV \int_{0}^{\infty} e^{-ux} g(ux) du \]

is the function we need for \( x > 0 \).

If we are frustrated by the fact that \( \mathcal{E}(x) \) is defined only for \( x > 0 \), and is not an analytic function in the complex plane, we can define it also there:

\[ \mathcal{E}(z) = \int_{0+ic}^{\infty+i\epsilon} e^{-uz} g(uz) du + \frac{i\pi}{z} e^{-K/z} \text{Res}_{x=K} g(x) \]

Obviously we can proceed in an analogous way if \( g(z) \) has more poles on the positive semiaxis. Let us, for the moment, assume it has only poles there.
We now ask how can we construct a sequence of approximations to \( \mathcal{E}(z) \) from (3). We have already pointed out that the direct application of PA to (3) will most probably fail, because we can expect that PA will diverge on the positive semiaxis. However, as we know that PA are particularly efficient in approximating functions in domains of their meromorphy \[5\], we can use PA to approximate \( g(z) \) from (4), i.e. we propose to construct \([M/N]_g(z)\) and approximate \( \mathcal{E}(z) \) by:

\[
\mathcal{E}_{M,N}(z) = \text{PV} \int_0^\infty e^{-u[M/N]_g(uz)}du
\]  

(10)

The convergence of PA in measure in the neighbourhood of the positive semiaxis (where we assumed \( g(z) \) to be meromorphic, and therefore we expect this type of convergence) guarantees us that (10) will converge to (8). We want to point out that the idea of combining PA with the Borel method was proposed quite a time ago \[6\],[7], but in a context where the Borel transform was regular on the positive semiaxis. Essentially the same concept was used in \[8\], where the Partial Padé Approximant \[9\] was used to predict a sum of the series for the Gell-Mann-Low function of the effective charge.

Before we consider a more general situation when \( g(z) \) has also branch points on the positive semiaxis, let us see how the method works for two examples from QCD.

3 Two QCD series with only poles on the positive semiaxis

First, we consider the Bjorken sum rule. It is known \[10\] that in the large-\( \beta_0 \) approximation it has only four simple poles in the Borel plane and therefore our prescription would be exact for all \([M/N]\) with \( M \leq 3 \) and \( N \leq 4 \). For realistic values of \( \beta_0 \), the perturbation series has been calculated up to 3rd order and there exists an estimate for the next coefficient \[11\]. It has been demonstrated in \[11\] that \([2/1]\) PA to the Borel transform of the truncated series for \( f(x) \) (we take \( N_f = 3 \)):

\[
f(x) = 1 - x - 3.58x^2 - 20.22x^3 - 130x^4
\]  

(11)

where \( f(x) \) is defined in:

\[
\int_0^\infty [g_1^p(x, Q^2) - g_1^a(x, Q^2)]dx = \frac{1}{6} |g_A| f(\alpha_s/\pi)
\]  

(12)

exhibits a pole at \( y = 1.05 \) (\( y = \frac{\beta_0 \alpha_s}{4 \pi} \)), while we expect poles at \( \pm 1, \pm 2 \) in the large-\( \beta_0 \) limit, as mentioned above. Therefore we believe that

\[
f(z) = 1 - z \text{PV} \int_0^\infty e^{-u[2/1](u\frac{\beta_0}{4}z)}du
\]  

(13)
is a reasonable approximation to \( f(z) \) (for the exact definition of \( S \) see [11]). We shall not discuss this example in more depth, but only remark that the value of \( \alpha_s(Q^2 = 3GeV^2) \) found this way is \( 0.371^{+0.075}_{-0.068} \).

The next example, which we want to discuss in detail, is the asymptotic series for the running coupling constant obtained from the static QCD potential for which we take the Richardson potential [12]. We follow notations and conventions of [13], and for more clarity we shall cite some formulae from this paper.

The Richardson potential in momentum space is:

\[
V_R(q) = -\frac{16\pi^2 C_F}{\beta_0 q^2 \ln(1 + q^2/\Lambda_R^2)}
\]  

and we use \( n_f = 3 \), therefore \( \beta_0 = 11 - 2/3n_f = 9 \), also \( \Lambda_R = 4 \) and \( C_F = 4/3 \). This example is very instructive because one can find the exact formula for the perturbative coupling in the position space:

\[
\bar{\alpha}_R(1/r) = \frac{2\pi}{\beta_0} \left[ 1 - \int_1^\infty \frac{du}{u \ln^2(u^2 - 1) + \pi^2} \right]
\]  

At the same time the formula for the coupling in momentum space is:

\[
\alpha_R(q) = \frac{4\pi}{\beta_0} \left[ \frac{1}{\ln(1 + q^2/\Lambda_R^2)} - \frac{\Lambda_R^2}{q^2} \right]
\]

From this, one can calculate the \( \beta \) function:

\[
\beta_R(\alpha_R) = q^2 \frac{\partial \alpha_R(q)}{\partial q^2} = -\frac{\beta_0}{4\pi} \alpha_R^2 + \frac{\beta_0}{4\pi} \left[ \frac{\beta_0}{4\pi} - \frac{\Lambda_R^2}{q^2} \right]^2
\]

On the other hand, one has (for any potential) the expansion:

\[
\bar{\alpha}_V(1/r) = \sum_{n=0}^{\infty} f_n \left( -\beta_V(\alpha_V) \frac{\partial}{\partial \alpha_V} \right)^n \alpha_V(q = 1/r')
\]

where \( r' = r e^{\gamma_E} \), and \( \gamma_E \) is Euler’s constant. \( f_n \)’s are coefficients of the expansion of:

\[
f(u) = \sqrt{\frac{\tan(\pi u)}{\pi u}} \exp \left[ \sum_{n=1}^{\infty} \frac{(2u)^{2n+1}}{2n+1} \zeta(2n+1) \right] = \sum_{n=0}^{\infty} f_n u^n
\]

For details see [13].

For later considerations it will be useful to observe that \( f(u) \) can also be written in a different form:

\[
f(u) = \frac{1}{1 - 2u} \prod_{k=1}^{\infty} \frac{1 + \frac{u}{k}}{1 - \frac{2u}{2k+1}}
\]
From this formula we can immediately see that \( f(u) \) has zeros at negative integer values of \( u \) and simple poles at half-integer positive values.

It is important to observe from (17) that \( \beta_R(\alpha_R) \) is not analytic at \( \alpha_R(q) = 0 \). The reason is that \( \alpha_R(q) \to 0 \) for \( q \to \infty \) and therefore:

\[
\beta_R(\alpha_R) = -\frac{\beta_0}{4\pi} \alpha_R^2 + \text{terms like } e^{-\frac{4\pi}{\beta_0 \alpha_R}}
\]  

(21)

Summing up, we see that we can get for \( \bar{\alpha}_R(1/r) \) the perturbation expansion when we neglect "higher twists":

\[
\bar{\alpha}_R^{\text{pert}}(1/r) = \sum_{n=0}^{\infty} \alpha_R(q) \left( \frac{\beta_0 \alpha_R(q)}{4\pi} \right)^n n! f_n
\]  

(22)

with \( q = 1/r' \). The direct calculation of PAs to this series confirms our expectations: the majority of zeros and poles of diagonal PAs \([M/M]\) (the same is the case for paradiagonal sequences of the type \([M \pm 1/M]\)) lie on the positive semiaxis and interlace:
We see that for large \( q \) (\( \alpha_R \) small), there will be difficulties in finding stable values for PAs, because of condensation of their zeros and poles.

When we now go to the Borel plane we get the series which is just:

\[
\alpha_R(q)f\left(\frac{\beta_0\alpha_R(q)}{4\pi}\right)
\] (23)

However we know already (see (20)) that \( f(u) \) has only poles on the positive semi-axis, and therefore we can try to sum (22) using the formula:

\[
\bar{\alpha}_R(1/r)_{M,N} = \frac{1}{z} PV \int_0^\infty e^{-u/z} [M/N] f(u) du \bigg|_{z=\frac{\beta_0\alpha_R(q)}{4\pi}}
\] (24)
We see that PAs to $f(u)$ actually reconstruct zeros and poles on the real axis.
and that there are many other complex zeros and poles drifting away from \( u = 0 \), most probably "simulating" the essential singularity of \( f(u) \) at \( u = \infty \).

Now we can see what values for (22) can one get from (24). We shall compare these values with the ones obtained in \([13]\) as the best partial sums (denoted by \( \bar{\alpha}_{R,N}(1/r) \)), and those calculated from formula (15), though one must keep in mind, that (15) gives the exact value of \( \alpha_R \) in position space, while we are here estimating the sum (22) which is (15) "minus higher twists".

We present below the case \( M = N \), but include also [2/3], as it is the lowest PA which gives already values quite close to the limit and uses only five coefficients of the expansion.

\[
\begin{array}{cccccc}
1/r[GeV] & 10 & 20 & 50 & 100 \\
\hline
[2/2] & .2903148980 & .2370475373 & .1814661174 & .1522256606 \\
[2/3] & .2710750452 & .222228306 & .1757241919 & .1497191873 \\
[3/3] & .2714196149 & .2235681574 & .1759161959 & .1498234840 \\
[4/4] & .2714564564 & .2234913019 & .1758530906 & .1497850862 \\
[5/5] & .2714137805 & .2234817444 & .1758530534 & .1497859540 \\
[6/6] & .2714097805 & .2234792391 & .1758723578 & .1497857339 \\
[7/7] & .2713988440 & .2234777131 & .1758524051 & .1497857952 \\
[8/8] & .2714007078 & .2234779029 & .1758523985 & .1497857906 \\
\bar{\alpha}_R(1/r) & .2714046 & .2218345 & .1746993 & .1491174 \\
\bar{\alpha}_{R,N}(1/r) & .2856 & .22262 & .17647 & .14868 \\
\end{array}
\]

\[
\begin{array}{ccccc}
1/r[GeV] & 10^5 & 10^4 & 10^5 & 10^6 \\
\hline
[2/2] & .09908701930 & .07409640462 & .05937036386 & .04957967229 \\
[2/3] & .09908856884 & .07413913414 & .05938321829 & .0495832635 \\
[3/3] & .09909570614 & .07413847053 & .05938281763 & .04958320088 \\
[4/4] & .09909193228 & .07413842675 & .05938289532 & .04958322765 \\
[5/5] & .09909214599 & .07413844576 & .05938289564 & .04958322732 \\
[6/6] & .09909214737 & .07413844662 & .05938289573 & .04958322732 \\
[7/7] & .09909214937 & .07413844659 & .05938289572 & .04958322732 \\
[8/8] & .09909214928 & .07413844654 & .05938289571 & .04958322732 \\
\bar{\alpha}_R(1/r) & .09901686 & .07413084 & .05938213 & .04958315 \\
\bar{\alpha}_{R,N}(1/r) & .098937 & .07413536 & .05938222 & .04958339 \\
\end{array}
\]

We see that \( \bar{\alpha}_R(1/r)_{M,M} \) converge when \( M \) grows, but not to the values of \( \bar{\alpha}_R \) - we attribute this to the difference made by "higher twists". In other words we
claim that the procedure we propose sums the series (22) well, which allows us to see clearly the difference between the perturbative solution - represented by this series - and the full solution (13) including also nonperturbative effects. We demonstrate, therefore, once again the fact that the perturbation series contains only a part of the information about the full solution and that the requirement that the solution must be real for positive values of the coupling constant is not sufficient to compensate for the information contained in "higher twists" terms.

4 Branch points in the Borel transform

If the Borel transform has a branch point at \( z = K \), instead of a pole, then the integral (5) for \( x \in (0, \infty) \) instead of (7) takes the form:

\[
\Phi(x) = \int_0^\infty e^{-u} \text{Re} g(ux) du \pm i \int_{K/\epsilon}^\infty e^{-u} \text{Im} g(ux) du
\]  

(25)

if \( g(z)(z - K) \) is finite for \( z \to K \) (what is a condition for the existence of (3). Again, we see that the second integral, which is equal to the imaginary part of \( \Phi(x) \), has all terms of the asymptotic expansion for \( x = 0^+ \) vanishing, and therefore it is the first integral which is of interest for us.

In the same way, as in the case of the simple pole, we can find an integral representation for the analytic function having the required asymptotic expansion (3) and being real on the positive semiaxis:

\[
\mathcal{E}(z) = \int_{0+it}^{\infty+i\epsilon} e^{-u} g(uz) du - \frac{1}{2iz} \int_{K}^{\infty} e^{-u/z}[g(u+i\epsilon) - g(u-i\epsilon)] du
\]  

(26)

These facts were also observed earlier [14], but we want to stress that \( \text{Re}\Phi(x) \) has the same asymptotic expansion at zero as \( \Phi(x) \) and therefore it cannot be reliably estimated by calculation of partial sums.

If we want now to use the same concept as before: to sum (4) using PAs, we must remember that they will most probably not converge on semiaxis \( x \epsilon (K, \infty) \). We conjecture, however, that if PAs to \( g(z) \) converge in measure arbitrarily close to positive semiaxis (where we expect a cut, "reconstructed" by PAs, should lie), then the integral:

\[
\mathcal{E}(z)_{M,N} = PV \int_0^\infty e^{-u} [M/N]_g(uz) du
\]  

(27)

will converge to \( \text{Re}\Phi(z) \) (see (25)) for \( z \approx 0 \).

To check a plausibility of this hypothesis, we try to calculate this way:

\[
F(x) = \text{Re} \int_0^\infty e^{-u/x} \log(1 - u) du
\]  

(28)
i.e. we approximate \( F(x) \) by:

\[
F_{M,N}(x) = PV \int_0^\infty e^{-u/x} u[M/N] \log(1-t)/t(u) du
\]  

(29)

As \( \log(1-t)/t \) is the Stieltjes function, all poles of PAs to it lie on the semiaxis \((1, \infty)\) and interlace with zeros [3],[4].

On the other hand, \( F(x) \) can easily be converted to a simple principal value integral:

\[
F(x) = -x PV \int_0^\infty \frac{e^{-u/x}}{1-u} du
\]  

(30)

We give below values of \( F_{M,N}(x) \) for few values of \( x \) and compare them with values obtained from a numerical integration of the last formula.

| \( x \) | .05 | .1  | .2  | .95 | 5   |
|--------|-----|-----|-----|-----|-----|
| [1/1]  | 0.0527903605 | 0.1128659958 | 0.275471870 | 0.409215955 | 0.049324951 |
| [1/2]  | 0.0527972269 | 0.1131155255 | 0.2731042382 | 0.8349862840 | -1.544989018 |
| [2/2]  | 0.0527977128 | 0.1131547428 | 0.2705616695 | 0.7678390728 | -1.080166535 |
| [2/3]  | 0.0527977828 | 0.1131540942 | 0.2703267712 | 0.6479952192 | -0.590917162 |
| [3/3]  | 0.0527977927 | 0.1131486878 | 0.2708042139 | 0.7437635764 | -1.199222773 |
| [3/4]  | 0.0527977949 | 0.1131464797 | 0.2708502503 | 0.7091822199 | -0.256031716 |
| [4/4]  | 0.0527977953 | 0.1131466717 | 0.2707469311 | 0.6971934572 | -0.961775112 |
| [5/5]  | 0.0527977953 | 0.1131470772 | 0.2707743167 | 0.7066673691 | -0.711782921 |
| [6/6]  | 0.0527977953 | 0.1131470109 | 0.2707637347 | 0.6701782542 | -0.586264408 |
| [7/7]  | 0.0527977953 | 0.1131470222 | 0.2707667730 | 0.7125737482 | -0.577295644 |
| [8/8]  | 0.0527977953 | 0.1131470201 | 0.2707662425 | 0.7110753552 | -0.621454057 |
| [9/9]  | 0.0527977953 | 0.1131470205 | 0.2707662164 | 0.7110505353 | -0.665706353 |
| [10/10]| 0.0527977953 | 0.1131470205 | 0.2707662706 | 0.7113684213 | -0.688595754 |
| [11/11]| 0.0527977953 | 0.1131470205 | 0.2707662537 | 0.7114624672 | -0.691851149 |

It should be noticed that starting from [8/8] the quadruple precision was necessary to obtain the above numbers.

## 5 Conclusions

We have proposed above to use PAs to sum the Borel transforms of the series appearing in QCD, and then to calculate Cauchy Principal Value of the Borel integral to obtain a function which has the given series as its asymptotic expansion at zero, and which is at the same time real on the positive semiaxis in the complex
coupling constant plane. The proposal is not entirely new [8], but we have pointed out that it produces values of the well defined analytic function, one of the variety of them having the same asymptotic expansion. We have also argued that the method should work not only in the case when the Borel transform has poles on the positive semiaxis, but also when it has branchpoints there. This latter point is illustrated by the very simple numerical experiment.

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