On the Self-Consistency of Scale-Setting Methods

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Abstract

We discuss various self-consistency conditions for scale-setting methods. We show that the widely used Principle of Minimum Sensitivity (PMS) is disfavored since it does not satisfy these requirements.

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Perturbative results in Quantum Chromodynamics (QCD) suffer from the well-known scale ambiguity problem \[1, 2, 3\]. That is, given a physical quantity
\[
R_N = r_0 \alpha^p(\mu) + r_1(\mu) \alpha^{p+1}(\mu) + \ldots + r_N(\mu) \alpha^{p+N}(\mu)
\] (1)
expanded to \(N\)-th order in a coupling constant \(\alpha(\mu)\), the renormalization scale \(\mu\) must be specified in order to obtain a definite prediction. Although the infinite series \(R_\infty\) is renormalization scale independent, at finite order the scale dependences from \(\alpha(\mu)\) and \(r_i(\mu)\) do not exactly cancel, leading hence to a scale ambiguity.

Various scale-setting procedures have been proposed in the literature:

1. **Fastest Apparent Convergence (FAC)** \[1\]
   This method chooses the renormalization scale \(\mu\) that makes the next-to-leading order coefficient vanish:
   \[
r_1(\mu) = 0.
\] (2)

2. **Principle of Minimum Sensitivity (PMS)** \[2\]
   This method chooses \(\mu\) at the stationary point of \(R\):
   \[
   \frac{dR_N}{d\mu} = 0.
\] (3)
   Beyond the next-to-leading order, PMS actually requires the optimization of scheme parameters in addition to the renormalization scale.

3. **Brodsky-Lepage-Mackenzie (BLM)** \[3\]
   We shall consider it here to be the condition of a vanishing \(N_f\) term in the next-to-leading order coefficient, where \(N_f\) the number of light-quark flavors. That is, if
   \[
r_1(\mu) = r_{10}(\mu) + r_{11}(\mu)N_f,
\] (4)

\[1\]Related to this subject is the scheme ambiguity problem. That is, we can choose \(\alpha\) in any scheme in the expansion of \(R_N\). However, as discussed in Ref. \[4\], the scheme ambiguity problem can be effectively reduced to the scale-ambiguity problem, in the sense that if we have a perfect scale-setting method, we can freely transform the coupling constant from one scheme to another.
where \( r_{10}(\mu) \) and \( r_{11}(\mu) \) are \( N_f \) independent, then BLM chooses the scale \( \mu \) given by the condition

\[
r_{11}(\mu) = 0. \tag{5}
\]

This prescription ensures that, as in quantum electrodynamics, vacuum polarization contributions due to fermion pairs are associated with the coupling constant \( \alpha(\mu) \) rather than the coefficients.

Due to the absence of all-order results in QCD, it is difficult to judge the performance of the various scale-setting methods. However, there are a number of self-consistency requirements that can shed some light into the reliability of these methods.

1. **Existence and Uniqueness of \( \mu \).**
   Clearly, it is desirable to have a scale-setting method that guarantees these two features.

2. **Reflexivity.**
   Given a coupling constant (or effective charge, see Ref. [1]) \( \alpha(\mu) \) specified at a scale \( \mu \), we can express it in terms of itself, but specified at another scale \( \mu' \):

   \[
   \alpha(\mu) = \alpha(\mu') - \frac{\beta_0}{4\pi} \log(\frac{\mu^2}{\mu'^2}) \alpha^2(\mu') + \cdots, \tag{6}
   \]

   where \( \beta_0 = 11 - 2N_f/3 \) is the first coefficient of the QCD beta function. If a scale-setting prescription is self-consistent, it should choose the unique value \( \mu' = \mu \) on the right-hand side. Notice that when \( \mu' \) is chosen to be \( \mu \), the above equation reduces to a trivial identity. This is a very basic requirement, since if \( \alpha(\mu) \) is known (say, experimentally measured for a range of scale \( \mu \)), and then we try to use the above equation to “predict” \( \alpha(\mu) \) from itself, any deviation of \( \mu' \) from \( \mu \) would lead to an inaccurate result due to the truncation of the expansion series.

3. **Symmetry.**
   Given two different coupling constants (or effective charges [1], or renormalization schemes) \( \alpha_1(\mu_1) \) and \( \alpha_2(\mu_2) \), we can express one of them in
terms of the other:

\[ \alpha_1(\mu_1) = \alpha_2(\mu_2) + r_{12}(\mu_1, \mu_2)\alpha_2^2(\mu_2) + \cdots, \quad (7) \]

\[ \alpha_2(\mu_2) = \alpha_1(\mu_1) + r_{21}(\mu_2, \mu_1)\alpha_1^2(\mu_1) + \cdots. \quad (8) \]

If a scale-setting method gives

\[ \mu_2 = \lambda_{21} \mu_1 \quad (9) \]

for the first series and

\[ \mu_1 = \lambda_{12} \mu_2 \quad (10) \]

for the second series, then this method is said to be symmetric if

\[ \lambda_{12} \lambda_{21} = 1. \quad (11) \]

This feature is desirable since it gives us a unique ratio between \( \mu_1 \) and \( \mu_2 \), irrelevant of which way we choose to expand the coupling constants.

4. **Transitivity.**

Given three different coupling constants \( \alpha_1(\mu_1) \), \( \alpha_2(\mu_2) \), and \( \alpha_3(\mu_3) \), we can establish the relation between \( \mu_1 \) and \( \mu_3 \) in two ways:

(a) Going through the extra scheme \( \alpha_2(\mu_2) \). That is, we can fix the scales in the two series

\[ \alpha_1(\mu_1) = \alpha_2(\mu_2) + r_{12}(\mu_1, \mu_2)\alpha_2^2(\mu_2) + \cdots, \quad (12) \]

\[ \alpha_2(\mu_2) = \alpha_3(\mu_3) + r_{23}(\mu_2, \mu_3)\alpha_3^2(\mu_3) + \cdots, \quad (13) \]

to obtain

\[ \mu_1 = \lambda_{12} \mu_2, \quad (14) \]

\[ \mu_2 = \lambda_{23} \mu_3, \quad (15) \]

and combine the last two expressions to get

\[ \mu_1 = \lambda_{12}\lambda_{23} \mu_3. \quad (16) \]

(b) Directly setting \( \mu_1 \) in terms of \( \mu_3 \) in the series

\[ \alpha_1(\mu_1) = \alpha_3(\mu_3) + r_{13}(\mu_1, \mu_3)\alpha_3^2(\mu_3) + \cdots \quad (17) \]

to get

\[ \mu_1 = \lambda_{13} \mu_3. \quad (18) \]
A scale-setting method is transitive if Eqs. (16) and (18) give the same result. That is,
\[ \lambda_{12} \lambda_{23} = \lambda_{13}. \]  
\( (19) \)

A scale-setting method that satisfies reflexivity, symmetry, and transitivity effectively establishes an equivalent relation among all the effective charges. This is a highly desirable feature since it guarantees that no matter how we move from one effective charge to another, we will always keep a consistent choice of scale.

In what follows we will consider the case of QCD with \( N_f \) massless quarks. It is straightforward to verify that the FAC and BLM criteria satisfy all the consistency requirements outlined above.

1. The existence and uniqueness of \( \mu \) are guaranteed, since the scale-setting conditions of FAC and BLM are simple linear equations in \( \log \mu^2 \). In fact, the next-to-leading coefficient \( r_1(\mu) \) in Eq. (1) has the form
\[ r_1(\mu) = (a + bN_f) + (c + dN_f) \log \mu^2, \]  
\( (20) \)
with \( a, b, c \) and \( d \) simple constants that are independent of \( N_f \). The solution given by FAC is
\[ \log \mu^2_{\text{FAC}} = -\frac{a + bN_f}{c + dN_f}, \]  
\( (21) \)
whereas the solution given by BLM is
\[ \log \mu^2_{\text{BLM}} = -\frac{b}{d}. \]  
\( (22) \)

2. Reflexivity is satisfied. In Eq. (6) both methods require the logarithm \( \log(\mu^2/\mu'^2) \) in the next-to-leading coefficient to vanish, hence
\[ \mu' = \mu. \]  
\( (23) \)

3. Symmetry is trivial since in Eqs. (\( \ref{eq:FAC} \)) and (\( \ref{eq:BLM} \)) we always have
\[ r_{12}(\mu_1, \mu_2) = -r_{21}(\mu_2, \mu_1). \]  
\( (24) \)
That is, the two next-to-leading order coefficients only differ by a sign. Thus, requiring one of them to vanish (FAC) is equivalent to requiring the other one to vanish, and requiring one of them to be \( N_f \)-independent is equivalent to requiring the other one to be \( N_f \)-independent.
4. Transitivity also follows in both cases. In FAC the scales $\mu_1$ and $\mu_2$ are chosen such that the next-to-leading order term vanishes:

\begin{align}
\alpha_1(\mu_1) &= \alpha_2(\mu_2) + O(\alpha_2^3), \\
\alpha_2(\mu_2) &= \alpha_3(\mu_3) + O(\alpha_3^3).
\end{align}

(25)

(26)

Substituting Eq. (26) into (25) we obtain

\begin{equation}
\alpha_1(\mu_1) = \alpha_3(\mu_3) + O(\alpha_3^3).
\end{equation}

(27)

Notice that this last equation does not contain the next-to-leading order term, either. Thus, the relationship between $\mu_1$ and $\mu_3$ is still given by the FAC condition (i.e., no next-to-leading order term), even when we have employed an intermediate scheme. For the BLM method we have a similar situation. If the scales $\mu_2$ and $\mu_3$ in the following two series

\begin{align}
\alpha_1(\mu_1) &= \alpha_2(\mu_2) + r_{12}(\mu_1, \mu_2)\alpha_2^2(\mu_2) + O(\alpha_2^3), \\
\alpha_2(\mu_2) &= \alpha_3(\mu_3) + r_{23}(\mu_2, \mu_3)\alpha_3^2(\mu_3) + O(\alpha_3^3),
\end{align}

(28)

(29)

are chosen by the BLM method, then $r_{12}(\mu_1, \mu_2)$ and $r_{23}(\mu_2, \mu_3)$ are independent of $N_f$. After replacing Eq. (29) into Eq. (28)

\begin{equation}
\alpha_1(\mu_1) = \alpha_3(\mu_3) + [r_{12}(\mu_1, \mu_2) + r_{23}(\mu_2, \mu_3)]\alpha_3^2(\mu_3) + O(\alpha_3^3),
\end{equation}

(30)

we see that the next-to-leading order coefficient will also be $N_f$ independent, since it is the sum of two $N_f$-independent quantities.

Now let us turn our attention to PMS. Unfortunately it does not satisfy any of the self-consistency conditions outlined previously.

To begin with, unlike the cases of FAC and BLM, in general there are no known theorems that guarantee the existence or the uniqueness of the PMS solution. Although for practical cases PMS does provide solutions, and when there are more than one solution usually only one of them lies in the physically reasonable region [2], these observations alone do not prove that PMS will be trouble-free for new processes.

Before analyzing the other self-consistency relations, let us perform first some preliminary calculations.
Given the QCD beta function for an effective charge $\alpha_1$:

$$\beta(\alpha_1) = \frac{d}{d \log \mu_1^2} \left( \frac{\alpha_1}{4\pi} \right) = -\beta_0 \left( \frac{\alpha_1}{4\pi} \right)^2 - \beta_1 \left( \frac{\alpha_1}{4\pi} \right)^3 - \cdots,$$  \hspace{1cm} (31)

where $\beta_0 = 11 - \frac{2}{3}N_f$ and $\beta_1 = 102 - \frac{28}{3}N_f$. To the next-to-leading order, $\alpha_1$ is implicitly given by the following equation:

$$\frac{1}{a_1} + \log \left( \frac{a_1}{1 + a_1} \right) = \tau_1,$$  \hspace{1cm} (32)

where $a_1 = \beta_1 \beta_0^{-1} \alpha_1 / 4\pi$, and $\tau_1 = \beta_0^2 \beta_1^{-1} \log(\mu_1^2 / \Lambda_1^2)$. (The scale $\Lambda_1$ is effectively the 't Hooft scale of $\alpha_1$. See Ref. \[5\].)

Given two effective charges $\alpha_1$ and $\alpha_2$ (or, $a_1$ and $a_2$), they are related by the perturbative series

$$a_1(\tau_1) = a_2(\tau_2) + (\tau_2 - \tau_1) a_2^2(\tau_2) + \cdots,$$  \hspace{1cm} (33)

where $a_2 = \beta_1 \beta_0^{-1} \alpha_2 / 4\pi$, and $\tau_2 = \beta_0^2 \beta_1^{-1} \log(\mu_2^2 / \Lambda_2^2)$. This is an equation of the form of Eq. (1) where the scale $\mu_2$ is to be chosen. PMS proposes the choice of $\mu_2$ (or equivalently, $\tau_2$) at the stationary point, i.e.:

$$\frac{d a_1}{d \tau_2} = 0 = \frac{d}{d \tau_2} \left[ a_2(\tau_2) + (\tau_2 - \tau_1) a_2^2(\tau_2) \right].$$  \hspace{1cm} (34)

From here we obtain the condition:

$$1 + a_2 = \frac{1}{2(\tau_1 - \tau_2)}.$$  \hspace{1cm} (35)

In order to obtain $\tau_2$ in terms of $\tau_1$, we must solve the last equation in conjunction with

$$\frac{1}{a_2} + \log \left( \frac{a_2}{1 + a_2} \right) = \tau_2.$$  \hspace{1cm} (36)

In Fig. 1 we present the graphical solution of the PMS scale-parameter $\tau_2$ as a function of the external scale-parameter $\tau_1$. 

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Notice that in the large momentum region \((\tau_1, \tau_2 \gg 1)\) we have

\[
\tau_2 \sim \tau_1 - \frac{1}{2}.
\] (37)

In terms of \(\mu_1\) and \(\mu_2\), the relation becomes

\[
\frac{\mu_2}{\Lambda_2} \sim \frac{\mu_1}{\Lambda_1} \exp(-\beta_1/4\beta_0^2). \] (38)

Let us now check the other self-consistency relations for PMS. For simplicity we will consider the large momentum kinematic region where the above approximation holds, although none of our conclusions will rely on this approximation.

Reflexivity is violated in PMS. When the PMS method is applied to Eq. (1), from Eq. (38) we obtain:

\[
\mu' \sim \mu \exp(-\beta_1/4\beta_0^2) \neq \mu. \] (39)

This is a severe drawback of the PMS method. When we use an effective charge to predict itself, the application of the PMS method would lead to an inaccurate result. If PMS cannot provide the optimum scale even in this simple situation, its reliability for other processes is very questionable.
Symmetry and transitivity are also violated in PMS. From Eq. (38) we know that in general:
\[ \lambda_{ij} = \frac{\mu_i}{\mu_j} \sim \frac{\Lambda_i}{\Lambda_j} \exp(-\beta_1/4\beta_2^2). \]  
(40)

This would mean that
\[ \lambda_{12}\lambda_{21} \sim \exp(-\beta_1/2\beta_2^2) \neq 1, \]  
(41)
\[ \lambda_{12}\lambda_{23} \sim \frac{\Lambda_1}{\Lambda_3} \exp(-\beta_1/2\beta_2^2) \neq \lambda_{13} \sim \frac{\Lambda_1}{\Lambda_3} \exp(-\beta_1/4\beta_2^2). \]  
(42)

That is, PMS does not satisfy the symmetry and transitivity conditions stated in Eqs. (33) and (39).

Hence, when we successively express one effective charge in terms of others, PMS would lead to inconsistent scale choices. We can only conclude that the PMS method in general does not provide the optimum scale, since an optimum scale-setting methods should satisfy all these self-consistency requirements.

Let us point out that adding the scheme-parameter optimization in PMS does not change any of the above conclusions. The inability of PMS to meet these self-consistency requirements resides in that the derivative operations in general do not commute with the operations of reflexivity, symmetry and transitivity.

Finally, let us briefly comment on the extended renormalization group formalism recently studied in Ref. [5]. In this formalism, the effective charges of two physical observables can be related by an evolution path on the hypersurface defined by the QCD universal coupling function \( a(\tau, \{c_i\}) \) [5], where \( \tau \) is the scale parameter and \( \{c_i\} \) are the scheme parameters. Given an initial effective charge \( a_{\text{init}} \) at the point \( (\tau_{\text{init}}, \{c_{\text{init}}\}) \), we can use the evolution equations [3, 5]
\[ \frac{\delta a}{\delta \tau} = \beta(a, \{c_i\}) = -a^2(1 + a + c_2a^2 + c_3a^3 + \cdots), \]  
(43)
\[ \frac{\delta a}{\delta c_n} = \beta(n)(a, \{c_i\}) = -\beta(a, \{c_i\}) \int_0^a dx \frac{x^{n+2}}{\beta^2(x, \{c_i\})}. \]  
(44)

to evolve \( a_{\text{init}} \) into a final effective charge \( a_{\text{final}} \) at the point \( (\tau_{\text{final}}, \{c_{\text{final}}\}) \).

As long as we stay inside an analytical region where the second partial deriva-

\[ ^2 \text{Due to the lack of knowledge of higher-order scheme parameter of the initial and final} \]
tatives exist and commute, the predicted value of \( a_{\text{final}} \) will not depend on the path chosen for the evolution.

In Fig. 2 we illustrate the paths that represent the operations of reflexivity, symmetry and transitivity. We can pictorially visualize that the evolution paths satisfy all these three self-consistency properties. A closed path starting and ending at the point \( A \) represents the operation of identity. Since the predicted value does not depend on the chosen path, if the effective charge at \( A \) is \( a_A \), after completing the path we will also end up with an effective charge \( a_A \). Similarly, if we evolve \( a_B \) at \( B \) to a value \( a_C \) at \( C \), we are guaranteed that when we evolve \( a_C \) at \( C \) back to the point \( B \), the result will be \( a_B \). Hence, the evolution equations also satisfy symmetry. Transitivity follows in a similar manner. Going directly from \( D \) to \( F \) gives the same result as going from \( D \) to \( F \) through a third point \( E \).

Summarizing, we have outlined a number of self-consistency conditions for scale-setting methods, and shown that FAC and BLM satisfy these requirements, whereas PMS does not. We have pictorially argued that the formalism based on the extended renormalization group equations satisfies effective charges, in practice we need to truncate the fundamental beta function \( \beta(a, \{ c_i \}) \) and solve \( a(\tau, \{ c_i \}) \) in a finite-dimensional subspace.
all these requirements for scale and scheme variation.

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