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# A Systematic All-Orders Method to Eliminate Renormalization-Scale and Scheme Ambiguities in PQCD

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We introduce a generalization of the conventional renormalization schemes used in dimensional regularization, which illuminates the renormalization scheme and scale ambiguities of pQCD predictions, exposes the general pattern of nonconformal $\{\beta_i\}$ terms, and reveals a special degeneracy of the terms in the perturbative coefficients. It allows us to systematically determine the argument of the running coupling order by order in pQCD in a form which can be readily automatized. The new method satisfies all of the principles of the renormalization group and eliminates an unnecessary source of systematic error.

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An important goal in high energy physics is to make perturbative QCD (pQCD) predictions as precise as possible, not only to test QCD itself, but also to expose new physics beyond the standard model. In this letter we present a systematic method which determines the argument of the running coupling order by order in pQCD, and which can be readily automatized. The resulting predictions for physical processes are independent of theoretical conventions such as the choice of renormalization scheme and the initial choice of renormalization scale. The resulting scales also determine the effective number of flavors at each order of perturbation theory. The method can be applied to processes with multiple physical scales and is consistent with QED scale setting in the limit $N_c \to 0$. The new method satisfies all of the principles of the renormalization group [1], and it eliminates an unnecessary source of systematic error.

The starting point for our analysis is to introduce a generalization of the conventional schemes used in dimensional regularization in which a constant $-\delta$ is subtracted in addition to the standard subtraction $\ln 4\pi - \gamma_E$ of the $\overline{\rm MS}$-scheme. This amounts to redefining the renormalization scale by an exponential factor; i.e. $\mu_\delta^2 = \mu_{\overline{\rm MS}}^2 \exp(\delta)$. In particular, the MS-scheme is recovered for $\delta = \ln 4\pi - \gamma_E$. The $\delta$-subtraction defines an infinite set of renormalization schemes which we call the $\delta$-$\mathcal{R}$enormalization ($\mathcal{R}_\delta$) scheme; since physical results cannot depend on the choice of scheme, predictions must be independent of $\delta$. Moreover, as all $\mathcal{R}_\delta$ schemes are connected by scale-displacements, the $\beta$-function of the strong QCD coupling constant $a = \alpha_s/4\pi$ in any $\mathcal{R}_\delta$-scheme is the same:

$$\mu_\delta^2 \frac{da}{d\mu_\delta^2} = \beta(a) = -a(\mu_\delta)^2 \sum_{i=0}^{\infty} \beta_i a(\mu_\delta)^i \ . \qquad (1)$$

The $\mathcal{R}_\delta$-scheme exposes the general pattern of nonconformal $\{\beta_i\}$-terms and it reveals a special degeneracy of the terms in the perturbative coefficients which allows us to resum the perturbative series. The resummed series matches the conformal series, which is itself free of any scheme and scale ambiguities as well as being free of divergent renormalon series. It is the final expression one should use for physical predictions. It also makes it possible to setup an algorithm for automatically computing the conformal series and setting the effective scales for the coupling constant at each perturbative order.

Consider an observable in pQCD in some scheme which we put as the reference scheme $\mathcal{R}_0$ (e.g. the $\overline{\rm MS}$-scheme which is the conventional one in the literature) with the following expansion:

$$\rho_0(Q^2) = \sum_{i=0}^{\infty} r_i(Q^2/\mu_0^2) a(\mu_0)^i \ , \qquad (2)$$

where $\mu_0$ stands for the initial renormalization scale and $Q$ is the kinematic scale of the process. The more general

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expansion with higher tree level power in $a$ can readily be derived [2] and does not change our conclusions and results. Since results in any $\mathcal{R}_\delta$ are related by scale displacements, we can derive the general expression for $\rho$ by using the displacement relation:

$$a(\mu_0) = a(\mu_\delta) + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\mathrm{d}^n a(\mu)}{(\mathrm{d}\ln\mu^2)^n}\,|_{\mu=\mu_\delta}\,(-\delta)^n\ , \qquad (3)$$

where we used $\ln\mu_0^2/\mu_\delta^2 = -\delta$. Then $\rho$ in $\mathcal{R}_\delta$ to order $a^4$ reads:

$$\begin{aligned}\rho_\delta(Q^2) =& r_0 + r_1 a_1(\mu_1) + (r_2 + \beta_0 r_1\delta_1) a_2(\mu_2)^2 \\ &+ [r_3 + \beta_1 r_1\delta_1 + 2\beta_0 r_2\delta_2 + \beta_0^2 r_1\delta_1^2] a_3(\mu_3)^3 \\ &+ [r_4 + \beta_2 r_1\delta_1 + 2\beta_1 r_2\delta_2 + 3\beta_0 r_3\delta_3 + 3\beta_0^2 r_2\delta_2^2 \\ &+ \beta_0^3 r_1\delta_1^3 + \frac{5}{2}\beta_1\beta_0 r_1\delta_1^2] a_4(\mu_4)^4 + \mathcal{O}(a^5)\ . \qquad (4)\end{aligned}$$

where $\mu_i = Qe^{\delta_i/2}$ and the initial scale is for simplicity set to $\mu_0 = Q$ and we defined $r_i(1) = r_i$. An artificial index was introduced on each $a$ and correspondingly on each $\delta$ to keep track of which coupling each $\delta$ term is associated to. This will be useful later. We emphasize that the choice $\mu_0 = Q$ is arbitrary and is not the final argument of the running coupling. The final effective scales must be independent of the initial renormalization scale.

In a conformal (or scale-invariant) theory, where $\{\beta_i\} = \{0\}$, the $\delta$ dependency vanishes in Eq.(4). Therefore, by absorbing all $\{\beta_i\}$ dependency into the running coupling at each order, we obtain a final result independent of the initial choice of scale and scheme. The use of $\mathcal{R}_\delta$ allows us to put this on formal grounds. From the explicit expression in Eq.(4) it is easy to confirm that

$$\frac{\partial\rho_\delta}{\partial\delta} = -\beta(a)\frac{\partial\rho_\delta}{\partial a}\ . \qquad (5)$$

To satisfy scheme-invariance of the physical prediction; i.e. $\partial\rho_\delta/\partial\delta = 0$, we must set the scales such that $\beta(a) = 0$. This is equivalent to setting the $\{\beta_i\}$-coefficients equal to zero and leads to the conformal series. Notice that this holds at *any* order in perturbation theory and is a *theoretical* requirement, different from the physical fact that the *all-orders* expression for $\rho$, being a physical observable, must be renormalization scale and scheme invariant; i.e. $\mathrm{d}\rho/\mathrm{d}\mu_0 = 0$. It should be emphasized that this is not a fixed point expression for $a$ but is a fully conformal requirement; the $\beta$-function must vanish identically. This proves the concept of the *principal of maximal conformality* [3–5] (PMC) to any order.

The expression in Eq.(4) exposes the pattern of $\{\beta_i\}$-terms in the coefficients at each order. Such pattern has recently been considered in Ref. [9] for the Crewther relations. The $\mathcal{R}_\delta$-scheme reveals its origin and its generality for any pQCD prediction. It is possible to infer even more from Eq.(4). By using the logic that there is nothing special about a particular value of $\delta$, we must conclude that some of the coefficients of the $\{\beta_i\}$-terms are degenerate; e.g. the coefficient of $\beta_0 a(Q)^2$ and $\beta_1 a(Q)^3$ must be equal. Forgetting about any reference scheme, the expression for $\rho$ in any scheme must be of the form:

$$\begin{aligned}\rho(Q^2) =& r_{0,0} + r_{1,0} a(Q) + [r_{2,0} + \beta_0 r_{2,1}] a(Q)^2 \\ &+ [r_{3,0} + \beta_1 r_{2,1} + 2\beta_0 r_{3,1} + \beta_0^2 r_{3,2}] a(Q)^3 \\ &+ [r_{4,0} + \beta_2 r_{2,1} + 2\beta_1 r_{3,1} + \frac{5}{2}\beta_1\beta_0 r_{3,2} + 3\beta_0 r_{4,1} \\ &+ 3\beta_0^2 r_{4,2} + \beta_0^3 r_{4,3}] a(Q)^4 + \mathcal{O}(a^5) \qquad (6)\end{aligned}$$

where $r_{i,0}$ are the conformal parts of the perturbative coefficients. The $\mathcal{R}_\delta$-scheme not only illuminates the $\{\beta_i\}$-pattern, but also exposes a *special degeneracy* of coefficients at different orders. We have checked that this degeneracy holds for several known results and it is trivially consistent with QED. A QCD example is provided in the end.

The expression in Eq.(4) reveals how the $\{\beta_i\}$-terms must be absorbed into the running coupling. The different $\delta_k$'s keep track of the power of the $1/\epsilon$ divergence of the associated diagram at each loop order in the following way; the $\delta_k^p a^n$-term indicates the term associated to a diagram with $1/\epsilon^{n-k}$ divergence for any $p$. Grouping together the different $\delta_k$-terms one recovers in the Abelian limit the dressed skeleton expansion. Resumming the series according to this expansion thus correctly reproduces the QED limit of the observable and matches the conformal series with running coupling constants evaluated at effective scales at each order.

Using this information from the $\delta_k$-expansion, it can be shown that the order $a(Q)^k$ coupling must be resummed into the effective coupling $a(Q_k)^k$, given by:

$$r_{1,0}a(Q_1) = r_{1,0}a(Q) - \beta(a)r_{2,1} + \frac{1}{2}\beta(a)\frac{\partial\beta}{\partial a}r_{3,2} + \cdots + \frac{(-1)^n}{n!}\frac{\mathrm{d}^{n-1}\beta}{(\mathrm{d}\ln\mu^2)^{n-1}}r_{n+1,n}\ , \qquad (7)$$

$$\vdots$$

$$r_{k,0}a(Q_k)^k = r_{k,0}a(Q)^k + r_{k,0}\ k\ a(Q)^{k-1}\beta(a)\left\{R_{k,1} + \Delta_k^{(1)}(a)R_{k,2} + \cdots + \Delta_k^{(n-1)}(a)R_{k,n}\right\}\ , \qquad (8)$$

which defines the PMC scales $Q_k$ and where we introduced

$$R_{k,j} = (-1)^j\frac{r_{k+j,j}}{r_{k,0}}\ , \quad \Delta_k^{(1)}(a) = \frac{1}{2}\left[\frac{\partial\beta}{\partial a} + (k-1)\frac{\beta}{a}\right]\ , \quad \cdots \qquad (9)$$

Eq.(8) is systematically derived by replacing the $\ln^j Q_1^2/Q^2$ by $R_{k,j}$ in the logarithmic expansion of $a(Q_k)^k$ up to the highest known $R_{k,n}$-coefficient in pQCD. The derivations are straightforward but tedious and will be given elsewhere [2]. The resummation can be performed iteratively using the renormalization group equation for $a$ and leads to the effective scales for an $NNNLO$ prediction:

$$\ln\frac{Q_k^2}{Q^2} = \frac{R_{k,1} + \Delta_k^{(1)}(a)R_{k,2} + \Delta_k^{(2)}(a)R_{k,3}}{1 + \Delta_k^{(1)}(a)R_{k,1} + \left(\Delta_k^{(1)}(a)\right)^2 (R_{k,2} - R_{k,1}^2) + \Delta_k^{(2)}(a)R_{k,1}^2} \ . \tag{10}$$

The final pQCD prediction for $\rho$ after setting the PMC scales $Q_i$ reads

$$\rho(Q^2) = r_{0,0} + r_{1,0}a(Q_1) + r_{2,0}a(Q_2)^2 + r_{3,0}a(Q_3)^3 + r_{4,0}a(Q_4)^4 + \mathcal{O}(a^5) \ , \tag{11}$$

Note that $Q_4$ remains unknown as it requires to know $r_{5,1}$ in the coefficient of $a^5$. In some cases, this might be known or estimated. This last ambiguity resides only in the highest order coupling constant and is negligible in practice.

It is easy to see that the leading order values of the effective scales are independent of the initial renormalization scale $\mu_0$. This follows since taking $\mu_0 \neq Q$ we must replace $R_{k,1} \to R_{k,1} + \ln Q^2/\mu_0^2$ and thus the leading order effective scales read $\ln Q_{k,\mathrm{LO}}^2/\mu_0^2 = R_{k,1} + \ln Q^2/\mu_0^2$, where $\mu_0$ cancels and Eq. (10) at LO is recovered. More generally the effective scales do not depend on the initial renormalization scale at any order. In practice, however, since the $\beta$-function is not known to all orders, higher order residual renormalization scale dependency will enter through the running coupling constant. This residual renormalization scale dependency is strongly suppressed in the perturbative regime of the coupling [10, 11].

The effective scales contain all the information of the non-conformal parts of the initial pQCD expression for $\rho$ in Eq.(6), which is exactly the purpose of the running coupling constant. The quotient form of Eq. (10) sums up an infinite set of terms related to the known $r_{j,k\neq 0}$ which appear at every higher order due to the special degeneracy. It is, however, not the full solution as this requires to know all $r_{j,k\neq 0}$-terms to all orders. The method systematically sums up all known non-conformal terms, in principle to all-orders, but is in practice truncated due to the limited knowledge of the $\beta$-function.

In earlier PMC scale setting [3–5], and its predecessor, the Brodsky-Lepage-Mackenzie (BLM) method [6–8], the PMC/BLM scales have been set by using a perturbative expansion in $a$ and only approximate conformal series have been obtained. Here, we have been able to obtain the conformal series exactly due to the revelation of the $\{\beta_i\}$-pattern by $\mathcal{R}_\delta$ and the effective scales have naturally become functions of the coupling constant through the $\beta$-function, in principle to all orders.

In many cases the coefficients in a pQCD expression for an observable is computed numerically and the $\{\beta_i\}$ dependency is not known explicitly. It is, however, easy to extract the explicit number of quark flavor $N_f$ dependency, since $N_f$ enters analytically in any loop diagram computation. To use the systematic method presented in this letter one must put the pQCD expression into the form of Eq.(6). Due to the special degeneracy in the coefficient of the $\{\beta_i\}$-terms, it turns out that the $N_f$ series is all that is needed to find the $r_{j,k}$ coefficients and to set the effective scales. This allows to automate the scale setting process algorithmically for pQCD predictions.

The general $N_f$-series of the $n$-th order coefficient in pQCD reads:

$$r_n = c_{n,0} + c_{n,1}N_f + \cdots + c_{n,n-1}N_f^{n-1} \ . \tag{12}$$

By inspection of Eq.(6) it is seen that there are exactly as many unknown coefficients in the $\{\beta_i\}$-expansion at the order $a^n$ as the $N_f$ coefficients, $c_{n,j}$. This is only realized due to the special degeneracy found in (6) through its $\mathcal{R}_\delta$ expression. The $r_{i,j}$ coefficients in Eq.(6) can thus be expressed in terms of the $c_{n,j}$ coefficients. This means that the $N_f$ terms can unambiguously be associated to $\{\beta_i\}$-terms and demonstrates PMC as the underlying principle of BLM scale setting. The relations between $c_{n,j}$ and $r_{i,j}$ are easy to derive and they transform the BLM scales into the correct PMC scales [2].

The automation process can be outlined as follows:

1. Choose any $\delta$-$\mathcal{R}$enormalization scheme and scale.
2. Compute the physical observable in pQCD and extract the $N_\mathrm{f}$ coefficients, $c_{k,j}$.
3. Find the $\beta_i$ coefficients, $r_{k,j}$ from the $c_{k,j}$ coefficients and compute the PMC scales, $Q_k$.
4. The final pQCD expression for the observable reads $\rho_{\mathrm{final}}(Q) = \sum_{k=0} r_{k,0}a(Q_k)^k$.

**Example of $e^+e^- \to$ hadrons.** The ratio for electron-positron annihilation into hadrons, $R^{e^+e^-\to\mathbf{h}}$, was recently computed to order $a^4$ [12] and can be shown to exactly match the generic form of Eq.(6). It can be derived by analytically continuing the Adler function, $D$, into the time-like region, with $D$ given by:

$$D(Q^2) = \gamma_{\mathrm{ph}}(a) - \beta(a)\frac{d}{da}\Pi(Q^2, a) \ , \tag{13}$$

where $\gamma_{\rm ph}$ is the anomalous dimension of the photon field, $\Pi$ is the vacuum polarization function and they are given by the perturbative expansions: $\gamma_{\rm ph}(a) = \sum_{n=0}^{\infty} \gamma_n a^n$ and $\Pi(a) = \sum_{n=1}^{\infty} \Pi_n a^n$. It is easy to show that to order $a^4$ the perturbative expression for $R^{e^+e^-\to \mathbf{h}}$ in terms of $\gamma_n$ and $\Pi_n$ reads:

$$\begin{aligned} R^{e^+e^-\to \mathbf{h}}(Q) = \gamma_0 + \gamma_1 a(Q) + [\gamma_2 - \beta_0\Pi_2] a(Q)^2 \quad (14) \\ + [\gamma_3 + \beta_1\Pi_2 + 2\beta_0\Pi_3 - \beta_0^2 \frac{\pi^2\gamma_1}{3}] a(Q)^3 \\ + [\gamma_4 + \beta_2\Pi_2 + 2\beta_1\Pi_3 + \beta_0\Pi_4 \\ - \frac{5}{2}\beta_0\beta_1\frac{\pi^2\gamma_1}{3} - 3\beta_0^2\frac{\pi^2\gamma_2}{3} - \beta_0^3\pi^2\Pi_2] a(Q)^4 \ . \end{aligned}$$

As expected, this expression has exactly the form of Eq.(6), with the coefficients: $r_{i,0} = \gamma_i$, $r_{i,1} = \Pi_i$, $r_{i,2} = -\frac{\pi^2}{3}\gamma_{i-2}$ and $r_{i,3} = -\pi^2\Pi_{i-2}$. Note that we here have knowledge of higher order coefficient, which allows us to set the effective scales $Q_1$, $Q_2$ and $Q_3$ to the NNNLO order, given by Eq.(10). It is worth noting that the Adler function $D$ itself has a much simpler $\{\beta_i\}$ structure. By convention the argument of $a$ is space-like, however, the $\pi^2$-terms appearing in $R^{e^+e^-\to \mathbf{h}}$ might be avoided by using a coupling constant with time-like argument, leading to a more convergent series [14].

The last unknown scale can in this case be estimated. It is to leading order given by $\ln \frac{Q_4^2}{Q^2} = -\frac{\Pi_5}{\gamma_4}$, where $\Pi_5$ is unknown, but it can be expressed in terms of coefficient among which all but one are known from the lower order coefficients [2]. It turns out that $Q_4 \sim Q$ which is the value we have used. The expression for the coefficient $\gamma_i$ and $\Pi_i$ can be found in Ref. [12], while the four-loops $\beta$-function is given in Ref. [13]. The final result in numerical form in terms of $\alpha = \alpha_s/\pi$ for QCD with five active flavors reads:

$$\begin{aligned} \frac{3}{11} R^{e^+e^-\to \mathbf{h}}(Q) = 1 + \alpha(Q_1) + 1.84\alpha(Q_2)^2 \\ - 1.00\alpha(Q_3)^3 - 11.31\alpha(Q_4)^4 \ . \quad (15) \end{aligned}$$

This is the most convergent result compared to all previous estimates, it is free of any scheme and scale ambiguities (up to strongly suppressed residual ones) and is to date the most exact estimate. To find numerical values for the effective scales, we must determine the asymptotic scale, $\Lambda$, of the running coupling by comparing with experimental results [15]:

$$\frac{3}{11} R^{e^+e^-\to \mathbf{h}}_{\rm exp}(\sqrt{s} = 31.6 \text{ GeV}) = 1.0527 \pm 0.0050 \ . \quad (16)$$

The asymptotic scale $\Lambda$ is derived by matching Eq.(15) with the experimental result and using a logarithmic expansion solution of the renormalization group equation for $a$ from which we find: $\Lambda_{\overline{\rm MS}} = 419^{+222}_{-168}$ MeV. Here we have used the $\overline{\rm MS}$ definition for the asymptotic scale for comparison with other estimates. The asymptotic scale of $\mathcal{R}_\delta$ can be taken to be the same for any $\delta$. The effective scales are found to be: $Q_1 = 1.3Q$ , $Q_2 = 1.2Q$, $Q_3 \approx 5.3Q$. The values are independent of the initial renormalization scale up to some residual dependency coming from the truncated $\beta$-function, which is less than the quoted accuracy on the numbers. This is illustrated in Fig. 1. For $Q_3$ we have taken the LO value, which is sufficient to get the conformal series at four loops, and is renormalization scale independent. Its higher order value has artificially strong residual renormalization scale dependency due to the large numerical value of $\Pi_4$ in QCD with five active flavors.

We have checked against the QED case, where $R^{e^+e^-\to \mathbf{h}}$ can be seen as the imaginary part of the QED four loop 1PI vacuum polarization diagram by the optical theorem, and find in this case nearly complete renormalization scale independence of all three scales to the NNNLO order due to the small value of the coupling constant. Numerically, we get for three (lepton) flavors:

$$\begin{aligned} \frac{1}{3} R^{e^+e^-\to \ell}_{\rm QED}(Q) = 1 + 0.24\alpha_e(Q_1) - 0.08\alpha_e(Q_2)^2 \\ - 0.13\alpha_e(Q_3)^3 + 0.05\alpha_e(Q_4)^4 \ , \quad (17) \end{aligned}$$

where $\alpha_e = e^2/4\pi$ and $\{\frac{Q_1}{Q}, \frac{Q_2}{Q}, \frac{Q_3}{Q}\} = \{1.1, 0.6, 0.5\}$.

For completness, we use our final result to predict the strong coupling constant at the scale of the Z-boson mass, $M_Z$, which reads:

$$\alpha_s(M_Z) = 0.132^{+0.010}_{-0.011} \ . \quad (18)$$

In this letter, we have shown that a generalization of the conventional $\overline{\rm MS}$-scheme is illuminating. It enables one to determine the general (and degenerate) pattern of nonconformal $\{\beta_i\}$-terms and to systematically determine the argument of the running coupling order by order in pQCD, in a way which is readily automatized. The resummed series matches the conformal series, in which no factorially divergent $n!\beta^n\alpha_s^n$ "renormalon" series appear and which is free of any scheme and scale ambiguities.

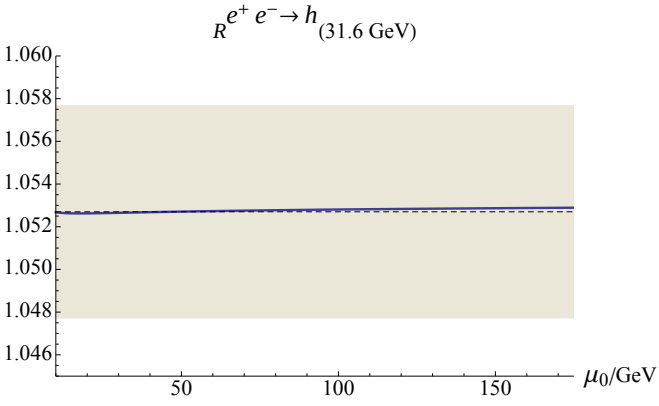


**FIG. 1:** The final result for $R^{e^+e^-\to \mathbf{h}}$ as a function of the initial renormalization scale (solid line), showing the initial scale-invariance of the final prediction up to strongly suppressed residual dependency. The shaded region is the experimental bounds with the central value given by the dashed line.

This is the final expression one should use for physical predictions. The method can be applied to processes with multiple physical scales and is consistent with QED scale setting in the limit $N_C \to 0$. The new method satisfies all of the principles of the renormalization group, including the principle of maximum conformality, and it eliminates an unnecessary source of systematic error.

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