Optimization for factorized quantities
in perturbative QCD

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Abstract:

Perturbative calculations of factorized physical quantities, such as moments of structure functions, suffer from renormalization- and factorization-scheme dependence. The application of the principle of minimal sensitivity to “optimize” the scheme choices is reconsidered, correcting deficiencies in the earlier literature. The proper scheme variables, RG equations, and invariants are identified. Earlier results of Nakkagawa and Niégawa are recovered, even though their starting point is, at best, unnecessarily complicated. In particular, the optimized coefficients of the coefficient function $C$ are shown to vanish, so that $C_{\text{opt}} = 1$. The resulting simplifications mean that the optimization procedure is as simple as that for purely-perturbative physical quantities.
1 Introduction

The application of the principle of minimal sensitivity \[1\] to the problem of factorization-scheme dependence has had a rather unfortunate history. The present author shares some of the blame, and this paper aims to make amends. The pioneering work by Politzer \[2\], which showed the way, was marred by a trivial algebraic error, seemingly showing that the optimization equations had no solution. The error was belatedly corrected in Ref. \[3\]. However, Ref. \[3\] is, in retrospect, insufficiently general beyond second order. The formulation of Nakkagawa and Niégawa (NN) in a series of papers \[4\]-\[7\] is, at best, unnecessarily complicated and creates spurious difficulties. However, NN’s optimization equations are actually equivalent to those we derive below. We discuss their work in Appendix A. Note that in Refs. \[2\]-\[7\] “b” has the opposite sign to ours.\[1\]

The prototypical factorization problem is in deep-inelastic lepton production, where a high-energy lepton collides with a proton, or other hadron, exchanging a virtual photon of large virtuality \(Q^2\). Neglecting power-suppressed terms, the \(n\)th moment, \( \int_0^1 \frac{dx}{x^n} F(x, Q) \), of the non-singlet proton structure function can be factorized into the form

\[
F_n(Q) = \langle O_n(M) \rangle C_n(Q, M),
\]

where \( \langle O_n(M) \rangle \) is an operator matrix element, \( C_n \) is a coefficient function, and \( M \) is some arbitrary “factorization scale.” (From now on the moment index \( n \) will be suppressed.)

The operator matrix element \( \langle O(M) \rangle \) has an \( M \) dependence given by its anomalous dimension

\[
\frac{M}{\langle O \rangle} \frac{d\langle O \rangle}{dM} \equiv \gamma_\circ.
\]

While \( \langle O(M) \rangle \) itself cannot be calculated perturbatively, its anomalous dimension, \( \gamma_\circ \), has a calculable perturbation series of the form

\[
\gamma_\circ(a) = -bg(a(1 + g_1a + g_2a^2 + \ldots)).
\]

The leading-order coefficient is written as \( -bg \) for later convenience. While \( g \) is invariant the other coefficients, \( g_1, g_2, \ldots \) are scheme-dependent. The expansion parameter, \( a = a(M) \), is the couplant in some arbitrary renormalization scheme (RS) with renormalization scale \( M \). Its \( M \) dependence is given by the \( \beta \) function:

\[
M \frac{\partial a}{\partial M} = \beta(a) = -ba^2(1 + ca + c_2a^2 + \ldots).
\]

The scheme-dependent coefficients \( c_2, \ldots \) can be regarded as RS labels \[1, 8\].

\[1\] Our notation follows Ref. \[8\], except that we now omit tildes on \( \Lambda \) and \( \rho_j \), which had merely emphasized a difference in definition from previous conventions. Tildes will be needed here for another purpose.
The coefficient function $C$ can be calculated as a perturbation series:

$$C(Q, M) = 1 + r_1 \tilde{a} + r_2 \tilde{a}^2 + \ldots,$$

(1.5)

where $\tilde{a}$ is the couplant of some other arbitrary RS – which can be different from the RS used to define $a$. It can have a different renormalization scale $\tilde{M}$, and different RS labels $\tilde{c}_2, \ldots$. (In the latter respect we differ from Ref. [3].) Perhaps the easiest way to understand that the RS’s for $a$ and $\tilde{a}$ can be distinct, without inconsistency, is to imagine that first both $\langle O \rangle$ and $C$ are calculated in the same RS and then a substitution $\tilde{a} = a(1 + v_1 a + v_2 a^2 + \ldots)$, with arbitrary $v_1, v_2, \ldots$, is made in the result for $C$. In terms of renormalization constants, the $Z_O$ constant needed for the renormalization of the operator $O$ (which is genuinely an infinite change of normalization) must be consistent between the calculations of $C$ and $\gamma_O$, but the reparametrization step – the substitution $a = Z_a a_{\text{bare}}$ and $\tilde{a} = \tilde{Z}_a a_{\text{bare}}$ in the bare forms of $\gamma_O$ and $C$, respectively – can involve distinct $Z_a$ and $\tilde{Z}_a$ renormalization constants.

Thus, what we shall call “RS/FS dependence” involves a choice of factorization scheme (FS), parametrized by $g_1, g_2, \ldots$ and two, independent, choices of RS for $a$ and $\tilde{a}$ that are labelled, respectively, by $\tau, c_2, c_3, \ldots$ and by $\tilde{\tau}, \tilde{c}_2, \tilde{c}_3, \ldots$, where

$$\tau \equiv b \ln(M/\Lambda), \quad \tilde{\tau} \equiv b \ln(\tilde{M}/\Lambda).$$

(1.6)

(See Appendix B for the definition of $\Lambda$. Without loss of generality, we may assume that the two renormalization prescriptions for $a$ and $\tilde{a}$ are defined so that their $\Lambda$ parameters are the same.)

Integrating Eq. (1.2), utilizing the $\beta$-function equation, gives

$$\langle O \rangle = (\text{const.}) \exp \left( \int_a^\infty dx \gamma_O(x) \right).$$

(1.7)

Note that the $M$ dependence of $\langle O \rangle$ comes solely from $a$ (whereas the $M$ dependence of $C$ comes solely from the $r_i$ coefficients). The constant of integration may be written as a constant $A$ defined by

$$\langle O \rangle = A \exp \left( \int_0^a dx \frac{\gamma_O(x)}{\beta(x)} - \int_0^\infty dx \frac{g x}{x^2(1 + c x)} \right),$$

(1.8)

where, as with the definition of $\Lambda$, the lower limit of $x \to 0$ in each integral produces a divergence that cancels between the two integrals. The normalization constant $A$ is not calculable from perturbation theory, but is RS/FS invariant, as shown in Ref. [3].

2 Second-order approximation

We first discuss second order, where all authors are in agreement. A second-order approximation corresponds to truncating the series for $\gamma_O, C$, and $\beta$ after two terms. The integrals in Eq. (1.8)
become
\[
\int_0^a dx \frac{-bgx(1 + g_1 x)}{-bx^2(1 + cx)} - \int_0^\infty dx \frac{gx}{x^2(1 + cx)}
\]
\[
= gg_1 \int_0^a dx \frac{1}{1 + cx} - g \int_a^\infty dx \left( \frac{1}{x} - \frac{c}{1 + cx} \right)
\]
\[
= g \left( \frac{g_1}{c} \ln(1 + ca) + \ln(ca) - \ln(1 + ca) \right),
\] (2.1)
which exponentiates to
\[
(ca)^g (1 + ca)^{-g(1-g_1/c)}.
\] (2.2)
Substituting in Eq. (1.1), one obtains the second-order approximation to \( F \) as
\[
F^{(2)} = A(ca)^g (1 + ca)^{-g(1-g_1/c)}(1 + r_1 \tilde{a}).
\] (2.3)
This approximant depends on RS/FS choices through three variables, \( \tau \), \( \tilde{\tau} \), and \( g_1 \). Partial differentiations of Eq. (2.3) yield
\[
\frac{1}{F^{(2)}} \frac{\partial F^{(2)}}{\partial \tilde{\tau}} = \frac{1}{(1 + r_1 \tilde{a})} \left( -\tilde{a}^2 (1 + c \tilde{a}) r_1 + \tilde{a} \frac{\partial r_1}{\partial \tilde{\tau}} \right),
\] (2.4)
\[
\frac{1}{F^{(2)}} \frac{\partial F^{(2)}}{\partial \tau} = -ga(1 + g_1 a) + \frac{\tilde{a}}{(1 + r_1 \tilde{a})} \frac{\partial r_1}{\partial \tau},
\] (2.5)
\[
\frac{1}{F^{(2)}} \frac{\partial F^{(2)}}{\partial g_1} = \frac{g}{c} \ln(1 + ca) + \frac{\tilde{a}}{(1 + r_1 \tilde{a})} \frac{\partial r_1}{\partial g_1}.
\] (2.6)
Self-consistency of perturbation theory requires these variations to be of order \( a^2 \). Noting that \( \tilde{a} = a(1 + O(a)) \), we see that
\[
\frac{\partial r_1}{\partial \tilde{\tau}} = 0, \quad \frac{\partial r_1}{\partial \tau} = g, \quad \frac{\partial r_1}{\partial g_1} = -g,
\] (2.7)
so that \( r_1 \) has the form
\[
r_1 = g(\tau - g_1 - \sigma_1(Q)),
\] (2.8)
where \( \sigma_1(Q) \) is an invariant \(^2\)

Substituting Eq. (2.7) back into Eqs. (2.4,2.6) and equating to zero produces the optimization conditions. Since \( \partial r_1/\partial \tilde{\tau} \) vanishes, the solution to the optimization equation (2.4) is simply
\[
r_{1}^{\text{opt}} = 0.
\] (2.9)
The second optimization equation, from (2.5), then reduces to
\[
\tilde{a} = a(1 + g_1 a),
\] (2.10)
\(^2\) The earlier literature is a bit sloppy at this point, as we discuss in section 4.
and (2.6) gives

\[ \ln(1 + ca) = c\tilde{a}. \]  (2.11)

Eliminating \( \tilde{a} \) between these last two equations gives us the optimal \( g_1 \) in terms of \( a \):

\[ g_1^{\text{opt}} = \frac{\ln(1 + ca) - ca}{ca^2}. \]  (2.12)

Also, from the integrated \( \beta \)-function ("int-\( \beta \)") equation (see Appendix B), at second order, we have

\[ \tau = \frac{1}{a} + c \ln \frac{ca}{1 + ca}. \]  (2.13)

Substituting for \( \tau \) and for \( g_1 \) in Eq. (2.8) and equating to zero, since \( r_1^{\text{opt}} = 0 \), we find

\[ \ln(1 + ca) - (ca)^2 \ln \frac{ca}{1 + ca} = ca (2 - a\sigma_1(Q)), \]  (2.14)

which determines the optimized \( a \) in terms of the invariant quantities \( c \) and \( \sigma_1(Q) \). Substituting back in Eq. (2.12) then fixes \( g_1^{\text{opt}} \). The final optimized result, from Eq. (2.3), is

\[ F^{(2)}_{\text{opt}} = A(ca)^g(1 + ca)^{-g(1 - g_1^{\text{opt}}/c)}. \]  (2.15)

Note that the optimization condition \( r_1^{\text{opt}} = 0 \) means that \( C_{\text{opt}} = 1 \), so that all perturbative corrections are effectively exponentiated and re-absorbed into the anomalous dimension by the optimization procedure. As we shall see later, this property holds at any order, as first noted by NN [5].

Also note that while the value of \( \tilde{a} \) (and hence \( \tilde{\tau} \)) is determined, it is not needed to obtain the result for \( F^{(2)}_{\text{opt}} \).

3 RG equations

As discussed above the RS/FS variables are \( \tau, c_j, \tilde{\tau}, \tilde{c}_j \), and the \( g_i \) coefficients. We now write down the RG equations expressing the fact that the physical quantity \( F \) is independent of all these variables. Symbolically, we have

\[ \frac{1}{F} \frac{\partial F}{\partial X} = 0, \]  (3.1)

where \( X \) stands for any of the set of variables \( \{\tau, c_j, \tilde{\tau}, \tilde{c}_j, g_j\} \).

Recalling the factorized form \( F = \langle O \rangle C \) of Eq. (1.1), and noting that \( \langle O \rangle \) is manifestly independent of \( \tilde{M} \), we see that

\[ \frac{1}{F} \frac{\partial F}{\partial \tilde{\tau}} = \frac{1}{C} \frac{\partial C}{\partial \tilde{\tau}}. \]  (3.2)
The same argument applies to the $\tilde{c}_j$ derivatives, since $\langle O \rangle$, while it depends on $a$ and its RS variables $\tau, c_j$, is manifestly independent of $\tilde{a}$ and its RS variables $\tilde{\tau}, \tilde{c}_j$. Thus, the first two RG equations have the familiar form

$$\left( \frac{\partial}{\partial \tilde{\tau}} \bigg|_{\tilde{a}} + \frac{\tilde{\beta}(\tilde{a})}{b} \frac{d}{d\tilde{a}} \right) C = 0, \quad "j=1"$$

$$\left( \frac{\partial}{\partial \tilde{c}_j} \bigg|_{\tilde{a}} + \tilde{\beta}_j(\tilde{a}) \frac{d}{d\tilde{a}} \right) C = 0, \quad j=2,3,\ldots,$$

where the first term collects dependence from the $r_i$ coefficients of $C$, while the second term collects the compensating dependence via $\tilde{a}$. (See Appendix B for the definition of the $\beta_j(a)$ functions.)

The other RG equations all take the form

$$\frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial X} + \frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial X} = 0,$$

where $X$ is any of the variables $\tau, c_j$ or $g_j$. The first term only involves dependence via the $r_i$ coefficients – indeed we are tempted to add “$|\tilde{a}$” (meaning “with $\tilde{a}$ held constant”) to the notation, to match Eqs. (3.3), (3.4), but it is unnecessary since $\tilde{a}$ is manifestly independent of $\tau, c_j$ and $g_j$. The second term can be evaluated as follows. In the case $X \rightarrow \tau$, we may simply use the definition of $\gamma_O$, Eq. (1.2), to get

$$\frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial \tau} = \gamma_O \frac{b}{b}.$$  (3.6)

For $X \rightarrow c_j$ we can first write

$$\frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial c_j} = \frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial c_j} \bigg|_{a} + \frac{1}{\langle O \rangle} \frac{d\langle O \rangle}{da} \frac{\partial a}{\partial c_j},$$

and then use Eq. (1.8) to obtain

$$\frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial c_j} = \int_{0}^{a} dx \gamma_o(x) \frac{b x^{j+2} + \gamma_o(a) \beta_j(a)}{\beta(a) \beta(x^2)}.$$  (3.8)

Although we return to this form later, for the present we follow NN and re-write it as

$$\frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial c_j} = \int_{0}^{a} dx \frac{\beta_j(x)}{\beta(x)} \gamma_o(x),$$

where $\gamma'_o(x) \equiv d\gamma_o/dx$. The equivalence to Eq. (3.8) can be shown by integrating by parts and then using the differential equation satisfied by the $\beta_j$ functions (see Appendix B). Finally, for $X \rightarrow g_j$ we find, from Eq. (1.8),

$$\frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial g_j} = -bg \int_{0}^{a} dx \frac{x^{j+1}}{\beta(x)}.$$  (3.10)
Thus, the RG equations, in addition to Eqs. (3.3, 3.4), are
\[ \frac{1}{C} \frac{\partial C}{\partial \tau} + \frac{\gamma_0}{b} = 0, \quad \text{"}_j=1" \] (3.11)
\[ \frac{1}{C} \frac{\partial C}{\partial c_j} + \int_0^a dx \frac{\beta_j(x)}{\beta(x)} \gamma'_0(x) = 0, \quad j=2,3,\ldots, \] (3.12)
\[ \frac{1}{C} \frac{\partial C}{\partial g_j} - bg \int_0^a dx x^{j+1} \frac{\beta_j(x)}{\beta(x)} = 0, \quad j=1,2,\ldots, \] (3.13)

As usual, the RG equations determine how the coefficients \( r_i \) must depend on the RS/FS variables. We now re-write the RG equations to facilitate finding these dependences. First, we use the series for \( \gamma_0 \) and \( C \):
\[ \gamma_0(a) = -bg \sum_{i=0} g_i a^{i+1}, \quad C = \sum_{i=0} r_i \tilde{a}^i, \] (3.14)
with \( r_0 \equiv g_0 \equiv 1 \). Second, we convert the \( \beta, \beta_j \) functions to the \( B, B_j \) functions of Appendix B (whose series begin \( 1 + \ldots \)). A third simplification, concerning the lower limit of the \( i \) summations, is discussed below. We obtain
\[ \sum_{i=1}^j \frac{\partial r_i}{\partial \tau} \tilde{a}^i - \tilde{a}^2 \tilde{B}(\tilde{a}) \sum_{i=1}^j ir_i \tilde{a}^{i-1} = 0, \] (3.15)
\[ \sum_{i=j+1}^k \frac{\partial r_i}{\partial \tilde{c}_j} \tilde{a}^i + \tilde{a}^{j+1} \tilde{B}_j(\tilde{a}) \sum_{i=1}^j ir_i \tilde{a}^{i-1} = 0, \] (3.16)
\[ \frac{1}{C} \sum_{i=1}^j \frac{\partial r_i}{\partial \tau} \tilde{a}^i - ga \sum_{i=0}^j g_i a^i = 0, \] (3.17)
\[ \frac{1}{C} \sum_{i=j}^k \frac{\partial r_i}{\partial \tilde{c}_j} \tilde{a}^i + \frac{g}{j-1} \int_0^a dx x^{j-1} \frac{B_j(x)}{B(x)} \sum_{i=0}^j (i+1) g_i x^i = 0, \] (3.18)
\[ \frac{1}{C} \sum_{i=j}^k \frac{\partial r_i}{\partial g_j} \tilde{a}^i + g \int_0^a dx x^{j-1} \frac{B(x)}{B(x)} = 0. \] (3.19)

The \( i \) summations of the \( \partial r_i/\partial X \) terms inherently begin with \( i = 1 \), but in the \( c_j \) and \( g_j \) equations, where the second term starts only at order \( a^j \), it is immediately evident that \( r_i \) cannot depend on \( c_j \) or \( g_j \) for \( i < j \). Thus, we may begin those \( i \) summations at \( i = j \). For the \( \tilde{c}_j \) equation a stronger result holds, since \( \partial r_i/\partial \tilde{c}_j \) must vanish for \( i = j \) as well as for \( i < j \). This observation is crucial for the “exponentiation theorem” proved in Sect. 5.

In \((k+1)\)-th order all the sums would go up to \( i = k \) only and the equations would only be satisfied, in an arbitrary RS/FS, up to remainder terms of order \( a^{k+1} \). The vanishing of all terms up to and including \( a^k \) fixes the RS/FS dependence of the \( r_i \) coefficients, and leads us to identify a set of invariants, \( \sigma_j \), as discussed in the next section.
4 Invariants

The scheme dependences of $r_1$ were already found in Eq. (2.7) and led us to the first invariant

$$\sigma_1(Q) = \tau - g_1 - \frac{r_1}{g}. \quad (4.1)$$

It is $Q$ dependent because $r_1$, when calculated from Feynman diagrams, will contain a term $-bg\ln(Q/M)$. One can view $\sigma_1(Q)$ as $b\ln(Q/\Lambda_F)$, where $\Lambda_F$ is a scale specific to the quantity $F$, but related, in an exactly calculable way, to the $\Lambda$ of some universal, reference RS. The earlier literature used an “invariant” $\kappa_1$ given by

$$\kappa_1 = r_1 + gg_1 + bg\ln(Q/M). \quad (4.2)$$

It is true that $\kappa_1$ is invariant under changes of FS and renormalization scale, with the explicit $g_1$ and $M$ dependences cancelling the implicit $g_1$ and $M$ dependences of $r_1$. Where $\kappa_1$ fails to be invariant is under a change of RS that leaves the renormalization scale $M$ unchanged, but changes the renormalization prescription, so that $a' = a(1 + v_1 a + \ldots)$, with some arbitrary $v_1$. Under such a transformation the $a^g$ factor in $\langle O \rangle$, see Eq. (2.2), becomes $(a')^g = a^g(1 + gv_1 a + \ldots)$, so the coefficient $r_1$ must become $r'_1 = r_1 - gv_1$ to leave $F = \langle O \rangle C$ invariant. Thus, $\kappa'_1 = \kappa_1 - gv_1$.

Since our $\sigma_1(Q)$ is

$$\sigma_1(Q) = b\ln(Q/\Lambda) - \kappa_1/g, \quad (4.3)$$

this change in $\kappa_1$ cancels with the change from $\Lambda$ to $\Lambda'$, by the Celmaster-Gonsalves [9] relation.

The higher invariants, $\sigma_2, \sigma_3, \ldots$, can be defined to be $Q$-independent. As with the $\rho_j$ invariants, it is convenient to define the $\sigma_j$’s so that they reduce to the $\beta$-function coefficients $c_j$ in “effective charge” schemes, defined by the RS/FS choices $g_j = 0, r_i = 0$. The invariants, so defined, depend on $\tau$ and $\tilde{\tau}$ only via the difference $\tilde{\tau} - \tau$ and have no dependence on $Q$ or $\Lambda$.

To find the invariants we will need the conversion between $\tilde{a}$ and $a$; either $\tilde{a} = a(1 + V_1 a + V_2 a^2 + \ldots)$ or its inverse

$$a = \tilde{a}(1 + \tilde{V}_1 \tilde{a} + \tilde{V}_2 \tilde{a}^2 + \ldots). \quad (4.4)$$

The $\tilde{V}_i$ coefficients can most easily be found from the relation between the $\beta$ functions: $\tilde{\beta}(\tilde{a}) = (d\tilde{a}/da)\beta(a)$. (In fact, the calculation mirrors that for the $\rho_i$ invariants in Ref. [8].) The first three coefficients are

$$\tilde{V}_1 = \tilde{\tau} - \tau,$$

$$\tilde{V}_2 = (\tilde{\tau} - \tau)^2 + c(\tilde{\tau} - \tau) - (\check{c}_2 - c_2),$$

$$\tilde{V}_3 = (\tilde{\tau} - \tau)^3 + \frac{5}{2}c(\tilde{\tau} - \tau)^2 + (-2\check{c}_2 + 3c_2)(\tilde{\tau} - \tau) - \frac{1}{2}(\check{c}_3 - c_3). \quad (4.5)$$
Note that the \( \tilde{V}'s \) do not only involve differences \( c_j - \tilde{c}_j \). It is true, though, that the \( V_i \) coefficients of the inverse relationship are obtained by exchanging all plain and tilde variables.

We now turn to a calculation of the invariant \( \sigma_2 \). Expanding Eqs. (3.15–3.19) in powers of \( a \) and \( \tilde{a} \) and using the above result for \( \tilde{V}_1 \), we can extract the self-consistency conditions. From the lowest-order terms we recover Eqs. (2.7) for \( r_1 \)'s derivatives, plus confirmation that \( r_1 \) does not depend on the other RS/FS variables \( (c_2, \tilde{c}_2, g_2) \). From the next-order terms we find

\[
\begin{align*}
\frac{\partial r_2}{\partial \tau} &= r_1, \\
\frac{\partial r_2}{\partial c_2} &= 0, \\
\frac{\partial r_2}{\partial g_1} &= -g \left(r_1 - \frac{c}{2} + \tilde{\tau} - \tau\right), \\
\frac{\partial r_2}{\partial g_2} &= -\frac{g}{2} (1 + g).
\end{align*}
\]

Integrating each of these equations individually is easy, but combining the results consistently is a little tricky. However, it is straightforward to check our result that \( r_2 \) has the form:

\[
r_2 = \frac{1}{2} \left( -gc_2 + gg_1 c + gg_2 - g_2^2 + 2g_1 r_1 + r_1^2 + \frac{r_1^2}{g} + 2r_1 (\tilde{\tau} - \tau) \right) + \text{const.},
\]

where the constant is independent of all the RS/FS variables. The constant can be conveniently written as \( \frac{g}{2} \sigma_2 \) so that the invariant \( \sigma_2 \) is given by

\[
\sigma_2 = c_2 + g_2 - g_1 c - g_2^2 + \frac{2r_2}{g} - 2g_1 r_1 - \frac{r_1^2}{g^2} (1 + g) - \frac{2r_1}{g} (\tilde{\tau} - \tau).
\]

An easier and more systematic way to calculate the \( \sigma_i \) invariants is to find them as the \( \rho_i \) invariants associated with the physical quantity

\[
\mathcal{D} \equiv \frac{Q}{F} \frac{dF}{dQ}.
\]

The perturbation series for \( \mathcal{D} \) can be found in terms of the \( C \) and \( \gamma_0 \) series in various ways. Perhaps the simplest is the following. First, note that all the \( Q \) dependence of \( F \) resides in the \( r_i \) coefficients of \( C \). For dimensional reasons such \( Q \) dependence can come only via the ratios \( Q/M \) and \( Q/\tilde{M} \). Thus,

\[
\mathcal{D} = \frac{Q}{C} \frac{dC}{dQ} = -\frac{1}{C} \left( M \frac{dC}{dM} + \tilde{M} \frac{\partial C}{\partial \tilde{M}} \right) + \gamma_0.
\]

The \( M \) dependence of \( C \) must cancel out with that of \( \langle \mathcal{O} \rangle \) in the product \( F = \langle \mathcal{O} \rangle C \), so that

\[
M \frac{dC}{dM} = -\frac{\langle \mathcal{O} \rangle}{\langle \mathcal{O} \rangle} \frac{d\langle \mathcal{O} \rangle}{dM} = -\gamma_0,
\]

while \( C \) is independent of \( \tilde{M} \), so that

\[
0 = \tilde{M} \frac{dC}{dM} = \tilde{M} \frac{\partial C}{\partial \tilde{M}} \bigg|_{\tilde{a}} + \beta(\tilde{a}) \frac{dC}{d\tilde{a}}.
\]
From these observations we see that
\[ D = \gamma_0 + \frac{\beta(\tilde{a})}{C} \frac{dC}{d\tilde{a}}. \]  
(4.13)
Thus, \( D \) is, in a sense, a “physicalized” version of \( \gamma_0 \).

Substituting in the above formula we find
\[ D = -bga(1 + g_1 a + g_2 a^2 + \ldots) + (-b\tilde{a}^2)(1 + c\tilde{a} + \ldots) \frac{(r_1 + 2r_2\tilde{a} + \ldots)}{(1 + r_1 \tilde{a} + \ldots)}. \]  
(4.14)
We could now expand out in terms of \( \tilde{a} \), converting \( a \) to \( \tilde{a} \) using Eq. (4.4). Alternatively, we can eliminate \( \tilde{a} \) and find the series expansion in terms of \( a \). The results are more compact in the \( a \) scheme:
\[ D = -bga(1 + r_1^a a + r_2^a a^2 + \ldots), \]  
(4.15)
with
\[ r_1^D = g_1 + r_1/g, \]
(4.16)
\[ r_2^D = g_2 + \frac{1}{g} (2r_2 + c r_1 - r_1^2 - 2r_1(\tau - \tilde{r})) , \]
(4.17)
and so on. Note that these coefficients are independent of the FS and independent of the tilde RS variables, with the explicit \( g_i \) and \( \tilde{r}, \tilde{c}_j \) dependences exactly cancelling with the implicit dependences from the \( r_i \) coefficients; see Eqs. (2.7), (4.6). Thus, the \( r_i^D \) coefficients only depend, in the usual way, on the RS variables \( \tau, c_j \) associated with \( a \).

As usual, we can construct the \( \rho_j \) invariants for the quantity \( D \):
\[ \rho_1^D(Q) = \tau - r_1^D, \]
(4.18)
\[ \rho_2^D = c_2 + r_2^D - c r_1^D - (r_1^D)^2, \]
(4.19)
and these coincide with the \( \sigma \)'s. Indeed, it is easy to see that the “effective-charge-type” RS/FS used in the definition of the \( \sigma \)'s corresponds to the usual effective-charge scheme for \( D \), so the equivalence of \( \rho_j^D \) to \( \sigma_j \) is true for all \( j \).

The calculation can be straightforwardly extended to higher orders. Defining
\[ \Delta \equiv \tau - \tau = b \ln(\tilde{M}/M), \quad s_i \equiv \frac{r_i}{g}, \]  
(4.20)
the first three invariants are
\[ \sigma_1(Q) = \tau - g_1 - s_1, \]
(4.21)
\[ \sigma_2 = c_2 + g_2 - g_1 c - g_1^2 + 2s_2 - 2g_1 s_1 - s_1^2(1 + g) - 2s_1 \Delta, \]
(4.22)
\[ \sigma_3 = c_3 + cg_2^2 + 4g_1^3 - 6g_1 g_2 + 2g_3 - 2c_2 g_1 + 6(c_2 - c_1) s_1 - 4c_1 g_1 s_1 \]
\[ + 12g_2^2 s_1 - 6g_2 s_1 - 5c s_1^2 - 2c gs_1^2 + 12g_1 s_1^2 + 6g g_1 s_1^2 + 4s_1^2 + 6s_3^3 \]
\[ + 2g_2^2 s_1^2 + 4c s_2 - 2g_1 s_2 - 12s_1 s_2 - 6g s_1 s_2 + 6s_3 \]
\[ +(12g_1 s_1 - 10c s_1 + 12s_1^2 + 6s_2^2 - 12s_2)\Delta + 6s_1 \Delta^2. \]
(4.23)
Using these formulas the values of the invariants can be found from Feynman-diagram calculations performed in any convenient RS/FS.

5 The exponentiation theorem

The \((k+1)\)-th order approximation is defined by truncating the series for \(C, \gamma_0, B,\) and \(\tilde{B}\). The resulting approximant, in general, will have a residual RS/FS dependence that is formally of order \(a^{k+1}\). The optimization conditions correspond to requiring the RG equations to be exactly satisfied, with no remainder. (To avoid notational clutter, we leave it understood that, henceforth, any RS/FS-dependent symbol \((a, \tilde{a}, r_i, \text{etc.})\) stands for the optimized value of that quantity.)

At second order we saw that the \(\tilde{\tau}\) optimization equation gave \(r_1 = 0\). In third order \((k = 2)\) the \(\tilde{\tau}\) equation (3.15), in which \(\partial r_2 / \partial \tilde{\tau} = r_1\), reduces to

\[
(1 + c\tilde{a} + \tilde{c}_2\tilde{a}^2)(r_1 + 2r_2\tilde{a}) - r_1 = 0. \tag{5.1}
\]

Also, the \(\tilde{c}_2\) equation (3.16), in which the \(\tilde{B}_2(\tilde{a})\) factor cancels out because \(\partial r_2 / \partial \tilde{c}_2 = 0\), becomes just

\[
r_1 + 2r_2\tilde{a} = 0. \tag{5.2}
\]

Substituting this back into the previous equation gives \(r_1 = 0\). Substituting \(r_1 = 0\) back into Eq. (5.2) then gives \(r_2 = 0\). The result generalizes to all orders, as first noted by NN.

**Theorem** (Nakkagawa and Niégawa [5])

The solution to the \(\tilde{\tau}\) and \(\tilde{c}_j\) optimization equations is

\[
r_1 = r_2 = \ldots = r_k = 0. \tag{5.3}
\]

Thus, \(C = 1\) in the optimal scheme, so that all perturbative corrections are effectively exponentiated and re-absorbed into the anomalous dimension \(\gamma_0\).

**Proof:** The \(\tilde{c}_j\) optimization equation follows from Eq. (3.16):

\[
\sum_{i=j+1}^{k} \frac{\partial r_i}{\partial \tilde{c}_j} \tilde{a}^i + \tilde{a}^{i+1} \frac{\tilde{B}_j(\tilde{a})}{j-1} \frac{dC}{d\tilde{a}} = 0, \tag{5.4}
\]

where \(dC/d\tilde{a} = \sum_{i=1}^{k} ir_i\tilde{a}^{i-1}\). Recall that all terms up to and including \(\tilde{a}^k\) must cancel in any RS, thus determining \(\partial r_i / \partial \tilde{c}_j\). By starting the sum at \(i = j + 1\) we have already used the fact that \(\partial r_i / \partial \tilde{c}_j\) must vanish for \(i < j\) and for \(i = j\), as noted at the end of Sect. 3.
We begin by considering the case \( j = k \). The first term vanishes, as there are no terms in the sum, so we find that in the optimal scheme

\[
\frac{dC}{d\tilde{a}} = 0. \quad (5.5)
\]

Next, consider the case \( j = k - 1 \). In any scheme, cancellation of the \( \tilde{a}^k \) terms requires

\[
\frac{\partial r_k}{\partial \tilde{c}_{k-1}} = -\frac{r_1}{k-2}. \quad (5.6)
\]

In the optimal scheme the left-hand side must vanish, since \( \frac{dC}{d\tilde{a}} \) vanishes in the optimization equation (5.4). Thus, in the optimal scheme, \( r_1 = 0 \). Proceeding to the case \( j = k - 2 \) we can find \( \frac{\partial r_k}{\partial \tilde{c}_{k-2}} \) as a sum of \( r_1c \) and \( r_2 \) terms. In the optimal scheme this must vanish, and since we already have \( r_1 = 0 \), we now find that \( r_2 = 0 \), too. We may then proceed to successively lower \( j \) cases to see that other \( r_i \)'s vanish. Finally, we reach \( j = 1 \), where we are dealing with the \( \tilde{\tau} \) equation, which gives us \( r_{k-1} = 0 \). Substituting back into \( \frac{dC}{d\tilde{a}} = \sum_{i=1}^{k} ir_i\tilde{a}^{i-1} = 0 \) then shows that \( r_k = 0 \).

6 The optimization equations

The fact that \( C = 1 \) in the optimal scheme allows us to simplify the remaining optimization equations, which follow from Eqs. (3.17–3.19) with the \( i \) summations truncated at \( i = k \).

Also, recalling that the \( B_j(a) \) functions are related to the \( I_j(a) \) integrals, one sees that the \( c_j \) equation involves

\[
I_{j,i}(a) \equiv (i + 1) \int_0^a dx x^i I_j(x). \quad (6.1)
\]

This can be simplified by interchanging the order of the two integrations:

\[
I_{j,i}(a) = (i + 1) \int_0^a dx x^i \int_0^x dy \frac{y^{j-2}}{B(y)^2} = \int_0^a dy \frac{y^{j-2}}{B(y)^2} \int_y^a dx (i + 1)x^i = \int_0^a dy \frac{y^{j-2}}{B(y)^2} (a^{i+1} - y^{i+1}), \quad (6.2)
\]

to give

\[
I_{j,i}(a) = a^{i+1}I_j(a) - I_{i+j+1}(a), \quad (6.3)
\]

which corresponds to going back to the form in Eq. (3.8) for \( \frac{1}{\langle O \rangle} \frac{\partial \langle O \rangle}{\partial c_j} \). Also note that the \( g_j \) optimization equations involve a related set of integrals

\[
J_j(a) \equiv \int_0^a dx x^{j-2} \frac{1}{B(x)}. \quad (6.4)
\]
Thus, the $\tau$, $c_j$, and $g_j$ optimization equations can be written as

\[
\sum_{i=1}^{k} \frac{\partial r_i}{\partial \tilde{\tau}} \tilde{a}^i - ga \sum_{i=0}^{k} g_i a^i = 0, \quad "j=1" \tag{6.5}
\]

\[
\sum_{i=j}^{k} \frac{\partial r_i}{\partial c_j} \tilde{a}^i + g \sum_{i=0}^{k} g_i I_{j,i}(a) = 0, \quad j=2,...,k \tag{6.6}
\]

\[
\sum_{i=j}^{k} \frac{\partial r_i}{\partial g_j} \tilde{a}^i + g J_{j+1}(a) = 0. \quad j=1,...,k \tag{6.7}
\]

In each of these equations the first term is a polynomial in $\tilde{a}$ that must precisely cancel out the terms up to and including $\tilde{a}^k$ present in the second term, if it were expanded out in a power series in $\tilde{a}$. In Ref \[8\] we used the notation $\mathbb{T}_n[G(a)]$ to mean “truncate the series for $G(a) = G_0 + G_1 a + \ldots$ immediately after the $a^n$ term” (i.e., $\mathbb{T}_n[G(a)] \equiv G_0 + G_1 a + \ldots + G_n a^n$).

Here we will need $\mathbb{T}_k$ as the equivalent operation in the expansion parameter $\tilde{a}$. Thus, we may re-write the equations (swapping the order of the two terms and dividing out a $g$ factor) as

\[
a \sum_{i=0}^{k} g_i a^i - \mathbb{T}_k[a \sum_{i=0}^{k} g_i a^i] = 0, \quad "j=1" \tag{6.8}
\]

\[
\sum_{i=0}^{k} g_i I_{j,i}(a) - \mathbb{T}_k[\sum_{i=0}^{k} g_i I_{j,i}(a)] = 0, \quad j=2,...,k \tag{6.9}
\]

\[
J_{j+1}(a) - \mathbb{T}_k[J_{j+1}(a)] = 0, \quad j=1,...,k \tag{6.10}
\]

However, note that the arguments of the $\mathbb{T}_k$’s are all functions of $a$, rather than $\tilde{a}$, so it is best to think of the $\mathbb{T}_k[G]$ operation in three stages (i) expand $G$ as series in $a$ up to $a^k$; (ii) convert $a$ to $\tilde{a}$ using Eq. \[4.24\], and (iii) re-expand as a series in $\tilde{a}$, and truncate after the $\tilde{a}^k$ term.

A further simplification results from the realization that, since $C = 1$, we do not need to know the optimized value of $\tilde{a}$; nor do we need to know the $\tilde{c}_j$’s or $\tilde{\tau}$: they do not enter into the optimized result for $F$, which just involves evaluating $\langle O \rangle$ in the optimal scheme. Thus, what we need to do is to take combinations of the optimization equations in which $\tilde{a}$ and the $\tilde{V}_i$’s cancel out. From the resulting equation combinations we can solve for the $g_j$ coefficients in terms of the “principal variables” $a, c_2, \ldots c_k$. (Note that the $I$ and $J$ integrals are functions of these principal variables.) Finally, we can use the invariants, $\sigma_i$ and $\sigma_1(Q)$, and the int-$\beta$ equation to determine the optimized result. Note that when $r_i=0$ the $\sigma_j$’s have exactly the same form as the usual $\rho_j$ invariants with $g_i$’s in place of $r_i$’s.

In the next section we illustrate the above observations in the case of third order.
7 Third-order approximation

In third order \((k = 2)\) we have four remaining optimization equations, in the variables \(\tau, c_2, g_1,\) and \(g_2\). From Eqs.\((6.8)\)–\((6.10)\) these are

\[
a(1 + g_1 a + g_2 a^2) - \dot{a} - (g_1 + \dot{V}_1)\dot{a}^2 = 0, \quad (\tau) \tag{7.1}
\]

\[
I_{2,0} + g_1 I_{2,1} + g_2 I_{2,2} - \frac{1}{2} \dot{a}^2 = 0, \quad (c_2) \tag{7.2}
\]

\[
J_2 - \dot{a} - \left(\frac{c}{2} + \dot{V}_1\right)\dot{a}^2 = 0, \quad (g_1) \tag{7.3}
\]

\[
J_3 - \frac{1}{2} \dot{a}^2 = 0. \quad (g_2) \tag{7.4}
\]

Taking the \(g_1\) equation minus the \(\tau\) equation cancels the \(\dot{a}\) terms and, not coincidentally, the \(\dot{V}_1\) terms, leaving

\[
J_2 - a(1 + g_1 a + g_2 a^2) + \left(\frac{c}{2} + g_1\right)\dot{a}^2 = 0. \tag{7.5}
\]

An \(\dot{a}^2\) term remains, but we can substitute from the \(g_2\) equation to obtain

\[
J_2 + (c + 2g_1)J_3 - a(1 + g_1 a + g_2 a^2) = 0. \tag{7.6}
\]

Taking the \(g_2\) equation minus the \(c_2\) equation cancels the \(\dot{a}^2\) terms, giving

\[
J_3 - (I_{2,0} + g_1 I_{2,1} + g_2 I_{2,2}) = 0. \tag{7.7}
\]

We may solve these last two equations for \(g_1, g_2\) in terms of the principal variables \(a, c_2\).

From the four original equations we have extracted just two equations that give us the \(g_1, g_2\) coefficients that we need. There are effectively two other equations that we can just ignore; they would determine \(\dot{a}\) and \(\dot{V}_1\) (which gives \(\dot{\tau}\) and, combined with the int-\(\beta\) equation of the tilde scheme, would then fix \(\dot{\epsilon}_2\), but we have no need to obtain values for these variables.

To relate the principal variables to \(Q\) and the invariants, we substitute the optimal-scheme quantities into the expressions for \(\sigma_2\) and \(\sigma_1(Q)\), combining the latter with the int-\(\beta\) equation to eliminate \(\tau\). In the optimal scheme, since \(r_i = 0\), the formula for \(\sigma_2\) reduces to

\[
\sigma_2 = c_2 + g_2 - g_1 c - g_1^2, \tag{7.8}
\]

which is the familiar form of a \(\rho_2\) invariant, but with \(g_i\)’s as the coefficients. Similarly, in the optimal scheme

\[
\sigma_1(Q) = \tau - g_1 = K^{(3)}(a) - g_1, \tag{7.9}
\]

where \(K^{(3)}(a)\) is the third-order approximation to the \(K(a)\) function of the int-\(\beta\) equation.
8 A simpler approach

In fact, there is a simpler approach that allows us to get directly to the equations determining the optimal \( g_i \)'s. Consider the physical quantity \( D \) defined in Eq. (4.9), which we showed is given by Eq. (4.13), so that \( D = \gamma O \) when \( C = 1 \). That suggests that we consider \( F \) in the form:

\[
F = A \exp \int_{0}^{a} dx \frac{D(x)}{\beta(x)},
\]

where “[0]” is a shorthand for the same “lower limit of 0 with subtraction of the suitable infinite scheme-independent constant,” as in Eq. (1.8). Formally, this expression for \( F \) is valid quite generally, and is independent of the RS used, so it satisfies RG equations saying that the total dependences on \( \tau \) and \( c_j \) all vanish. What we are doing in RS/FS optimization is equivalent to a normal RS optimization applied to \( F \), except that the approximants being optimized are not truncations of the perturbation series for \( F \), but are approximants formed by truncating the perturbation series for \( D \) and \( \beta \). That is, the \((k+1)\)-th approximant to \( F \) is given by substituting

\[
D(x) = \sum_{i=0}^{k} r_i^p x^{i+1}, \quad \beta(x) = -bx^2 \sum_{j=0}^{k} c_j x^j
\]

into Eq. (8.1). The optimization equations follow from requiring the \( \tau \) and \( c_j \) derivatives to vanish. (Note that when we take such derivatives the infinite constant plays no role and the “[0]” lower limit can safely be replaced by 0, since the resulting integrals converge.) For \( \tau \) we have

\[
0 = \frac{1}{F} \frac{\partial F}{\partial \tau} = \frac{\partial a}{\partial \tau} \frac{D(a)}{\beta(a)} + \int_{0}^{a} dx \left( \frac{\partial D}{\partial \tau} \right) |_{x} \frac{1}{\beta(x)} = \frac{1}{b} \left( D(a) - \sum_{i=1}^{k} \frac{\partial r_i^p}{\partial \tau} J_{i+1} \right),
\]

while for \( c_j \)

\[
0 = \frac{1}{F} \frac{\partial F}{\partial c_j} = \frac{\partial a}{\partial c_j} \frac{D(a)}{\beta(a)} + \int_{0}^{a} dx \left( \frac{\partial D}{\partial c_j} \right) |_{x} \frac{1}{\beta(x)} + \frac{D(x)}{\beta(x)^2} bx^{j+2} \left( -D(a) I_j - \sum_{i=j}^{k} \frac{\partial r_i^p}{\partial c_j} J_{i+1} + \sum_{i=0}^{k} r_i^p I_{i+j+1} \right).
\]

Substituting the series form for \( D(a) \) leads to

\[
- \sum_{i=1}^{k} \frac{\partial r_i^p}{\partial \tau} J_{i+1} + \sum_{i=0}^{k} r_i^p a^{i+1} = 0,
\]

\[
\sum_{i=j}^{k} \frac{\partial r_i^p}{\partial c_j} J_{i+1} + \sum_{i=0}^{k} r_i^p I_{j,i} = 0.
\]
where \( I_{j,i}(a) = a^{i+1}I_j(a) - I_{i+j+1}(a) \) arises from the first and third terms of Eq. (8.4).

The derivatives \( \partial r_i^D/\partial \tau \) and \( \partial r_i^D/\partial c_j \) are the usual RS dependences of perturbative coefficients \([1, 8]\), and can be quickly found from the expressions for the \( \rho_i^p \) invariants. Thus,

\[
\frac{\partial r_1^D}{\partial \tau} = 1, \quad \frac{\partial r_2^D}{\partial \tau} = c + 2r_1^D, \quad \frac{\partial r_2^D}{\partial c_2} = -1. \tag{8.7}
\]

Using these results, and recalling that in the FS/RS optimal scheme the optimized \( r_i^D \)'s equal the optimized \( g_i \)'s, the reader can quickly check that at 3rd order \( (k = 2) \) Eqs. (8.5) and (8.6) lead directly to Eqs. (7.6) and (7.7).

At 4th order \( (k = 3) \) the \( \tau, c_2, c_3 \) equations reduce to

\[
J_2 + (c + 2g_1)J_3 + (c_2 + 2cg_1 + 3g_2)J_4 - a(1 + g_1a + g_2a^2 + g_3a^3) = 0, \tag{8.8}
\]

\[
J_3 + 2g_1J_4 - (I_{2,0} + g_1I_{2,1} + g_2I_{2,2} + g_3I_{2,3}) = 0, \tag{8.9}
\]

\[
\frac{1}{2}J_4 - (I_{3,0} + g_1I_{3,1} + g_2I_{3,2} + g_3I_{3,3}) = 0. \tag{8.10}
\]

We have explicitly checked that these are indeed the equations one would obtain from appropriate combinations of Eqs. (6.8), (6.9), (6.10).

### 9 Conclusions and outlook

The optimization approach to the problem of RS/FS dependence is now, we believe, on a firm footing. It is far less daunting than it might appear at first sight. There are \( 3k \) scheme variables at \( (k + 1) \)-th order and \( k \) coefficients, \( r_i \). However, \( k \) of the optimization equations lead to \( r_1 = \ldots = r_k = 0 \), so that \( C = 1 \); another \( k \) variables \((\tilde{\tau}, \tilde{c}_2, \ldots, \tilde{c}_k)\) then need not be solved for. That leaves \( k \) combinations of optimization equations that can be solved for \( g_1, \ldots, g_k \) in terms of the “principal variables” \( a, c_2, \ldots, c_k \). In fact, these equations can be obtained more directly by the approach in the last section. By substituting in the expressions for the invariants, one can then solve for all the needed quantities. The last step will require an iterative algorithm, as in ordinary optimization \([8]\).

Our results have applications to various quantities, such as charmonium decays to hadrons, \( B \) decays to charmonium, or Higgs boson decay to hadrons: These quantities have a factorized form involving the wavefunction at the origin or, in the last case, the quark masses. For applications involving parton distribution functions and fragmentation functions there is more work to be done. We have only considered the non-singlet case; the flavour-singlet case involves matrices describing quark-gluon mixing. Also, our analysis has used the language of structure-function moments, which is convenient theoretically since it reduces a convolution integral to a simple
product. However, phenomenologically, it seems preferable to deal directly with the parton distributions using parton-evolution (DGLAP) equations. It would be valuable to see if our moments-based approach can be reformulated in that language and put into practice.

We end with a plea to recognize of the importance of this effort. When QCD was young, the use of phenomenological, *ad hoc* choices was excusable, perhaps even necessary to make progress. Now that the theory is mature we cannot go on using arbitrary renormalization prescriptions and blind guesses at the “right” renormalization and factorization scales (which don’t even exist, since it is only the ratios of $M$ and $\tilde{M}$ to the prescription-dependent $\Lambda$ that matter). If “precision QCD” is to be a valid scientific enterprise, it must be based on a systematic treatment of RS/FS ambiguities, with a respect for RG invariance at its core.
Appendix A: Discussion of the work of NN

In this appendix we critique the work of Nakkagawa and Niégawa (NN) [4]-[7] and outline why, nevertheless, their optimization equations are equivalent to ours. Note that their “µ” corresponds to our ˜M (and their “b” is the opposite sign to ours). Their ˜a is the same as ours, but their a is somehow supposed to explicitly depend on both M and ˜M. They write a = a(µ, ξ) where ξ = M/µ. It is never clear quite how this object is defined. Because of its supposed dependence on two scales, NN associate it with two β functions, whose coefficients are supposed to depend on ξ. We find this rather odd; it might not be wrong, but it certainly creates difficulties without gaining any generality. In our approach the couplant a is a normal coupitant, with a renormalization scale M, in a RS labelled by τ ≡ b ln(M/Λ),c2,c3,… This RS is distinct from, and independent of, the tilde RS used for ˜a, whose scale is ˜M and whose scheme labels are ˜τ, ˜c2, ˜c3,… Along with FS labels g1,g2,… these form the complete set of RS/FS labels, and variation of any one label, in a partial derivative, is made holding the other labels constant. Thus, there is no question of cj’s “depending” on M or ˜M or their ratio.

For NN the integration of their two β-function equations for “a(µ, ξ)” is problematic [5, 6], because of a dependence on the integration path. Later [7] they claimed to have resolved this problem, and made the ξ dependence of their cj’s go away. In our view, this dependence and the integration-path problem should never have been there in the first place!

NN’s analysis involves a somewhat mysterious variable Φ, which it seems must actually be, in their notation, b ln(M/µ). In our notation that means Φ = −b ln(M/˜M) = ˜τ − τ. Provided that we make this identification, we find that their equations (Eqs. (18a-e) of Ref. [5]) are equivalent to ours. Apart from straightforward conversion of notation we need to recognize that they work with variables µ and Φ, etc., while we work with ˜M = µ and M (related to ˜τ and τ, respectively). Thus their ∂/∂Φ is at constant µ and coincides with our −(1/b)M∂/∂M = −∂/∂τ: However, their µ∂/∂µ is at constant Φ and so corresponds to our ˜M∂/∂˜M + M∂/∂M = b(∂/∂˜τ + ∂/∂τ). Hence, their optimization equation associated with µ is a sum of our ˜τ and τ optimization equations.

Notwithstanding our criticisms, NN deserve praise for arriving at the correct optimization equations, and they were correct to criticize Refs. [2, 3]’s formulation as insufficiently general. The applications of their results, pursued with Yokota [10], are valid and important. In particular, they show how optimization naturally resolves the issue that, in a naively fixed scheme, the perturbative coefficients for the nth moment would grow like ln n2.
Appendix B: $\beta(a)$ and $\beta_j(a)$ functions

For the reader’s convenience we list here some key formulas from Refs. [1, 8]. The integrated form of the $\beta$-function equation, referred to as the “int-$\beta$” equation, is

$$
\tau \equiv \ln(M/\Lambda) = \lim_{\delta \to 0} \left( \int_{\delta}^{a} \frac{dx}{\beta(x)} + C(\delta) \right) \equiv K(a),
$$

(B.1)

with

$$
C(\delta) \equiv \int_{\delta}^{\infty} \frac{dx}{bx^2(1+cx)}.
$$

(B.2)

The $\beta_j$ functions, defined as $\partial a/\partial c_j$, are given by

$$
\beta_j(a) = -b\beta(a) \int_{0}^{a} \frac{x^{j+2}}{\beta(x)^2}.
$$

(B.3)

Their series expansions begin at order $a^{j+1}$ so it is convenient to define $B_j(a)$ functions which begin $1 + O(a)$:

$$
B_j(a) \equiv \frac{(j-1)}{a^{j+1}} \beta_j(a).
$$

(B.4)

For $j = 1$ it is natural to define

$$
B_1(a) \equiv B(a) = \frac{\beta(a)}{-ba^2} = 1 + ca + c_2a^2 + \ldots = \sum_{i=0}^{\infty} c_i a^i,
$$

(B.5)

with the convention that $c_0 \equiv 1$ and $c_1 \equiv c$. Equation (B.3) can then be re-written as

$$
B_j(a) = \frac{(j-1)}{a^{j+1}} B(a) I_j(a),
$$

(B.6)

where

$$
I_j(a) \equiv \int_{0}^{a} \frac{x^{j-2}}{B(x)^2}.
$$

(B.7)

(Note that this formula for $B_j(a)$ even holds for $j = 1$ if the r.h.s. is interpreted as the limit $j \to 1$ from above.)

Differentiating Eq. (B.3) leads to

$$
\beta'_j(a) \beta(a) - \beta'(a) \beta_j(a) = -ba^{j+2},
$$

(B.8)

where here the prime indicates differentiation with respect to $a$, regarding the coefficients $c_j$ as fixed.
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