WEIGHTED ASYPMTOTIC PADÉ APPROXIMANT PREDICTIONS OF THE 4-LOOP AND 5-LOOP QCD AND SQCD BETA-FUNCTIONS WITH ERROR ESTIMATES.

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CHAPTER 1

INTRODUCTION

1.1 INTRODUCTION

The method of Padé Approximants is well known from statistical mechanics [1], but the application of this method to perturbative quantum field theories is a recent innovation. The power of this application lies in the ability to "feel" the effects of not only lower-order terms, as is the case in any perturbative calculation, but also the higher-order terms.

I will show that for the function

$$\frac{\ln(1+x)}{x} = 1 - \frac{1}{2}x + \frac{1}{3}x^2 - \frac{1}{4}x^3 + \cdots = \sum_{n=0}^{\infty}(-1)^n \frac{1}{n+1}x^n \qquad (1.1)$$

the [N/M] Padé converges to the actual value more rapidly, for a given x, than the partial sums. In fact, the partial sums fluctuate quite noticeably while the Padé converges to within a few percent on only four or five terms.

The number of Feynman diagrams involved in the exact calculation of given terms of a β-Function is expected to diverge factorially. The computation of the 5-Loop QCD β coefficient would require the evaluation of over 1 million Feynman diagrams! So the need for a less exhaustive calculation is clear. While it is possible that progress in computer technology and computational theory will someday offer a means to perform these exact calculations, we have an immediate desire to know these coefficients.

In this paper I will present my method for making an approximation of this coefficient as well as comparisons at lower orders. I am confident that the remarkable accuracy of the 4-Loop predictions will also be seen at the 5-Loop order, should the exact calculation ever be performed. I will also present a method which will lead

to reasonable error estimates for these 5-Loop predictions. Using the ϕ^4 theory as a guide, I can derive error bars based on the radius of curvature of the APAP; after demonstrating the effectiveness of this method at the 4-Loop level, I will present the results for the 5-Loop predictions.

When the LHC (Large Hardon Collider) at CERN starts running, it is expected that one of the results it finds will be a much more accurate measurement of α_s than exists now. If this measurement is accurate enough, it can be used to test the validity of the predictions made in this paper.

CHAPTER 2

Padé Formalism

Assume we know the first several terms of a series

$$S(x) = \sum_{n=0}^{\infty} s_n x^n \tag{2.1}$$

and let us define the $[N/M]$ Padé Approximant to be the rational function

$$[N/M] = \frac{a_0 + a_1 x + a_2 x^2 + \cdots + a_N x^N}{b_0 + b_1 x + b_2 x^2 + \cdots + b_M x^M} \equiv \frac{P_N(x)}{Q_M(x)}. \tag{2.2}$$

We equate the first $N + M$ terms of $S(x)$ to the Padé Approximant so that we can rewrite as

$$S(x) = [N/M] + \sum_{n=N+M+1}^{\infty} s_n x^n \tag{2.3}$$

If we now neglect terms of order $N + M + 2$ and higher, we can multiply through by $Q_M(x)$ and have

$$a_0 + a_1 x + a_2 x^2 + \cdots + a_N x^N =$$

$$(b_0 + b_1 x + b_2 x^2 + \cdots + b_M x^M)(s_0 + s_1 x + s_2 x^2 + \cdots + s_{N+M+1} x^{N+M+1}) \tag{2.4}$$

from which we can construct any number of simultaneous equations by increasing either N or M and letting $a_i = 0 \ \forall i > N$. These equations, however, will form an increasingly underdetermined system as we go to higher terms since by assumption we only know a finite number of terms in $S(x)$. So to keep the system within one degree of being fully determined, we will only allow one unknown to be introduced. We follow the convention that $b_0 \equiv 1$ and construct $N + M + 1$ equations from which we can solve for the unknowns a_i and b_i. For example, say we know only the

coefficients of the series $S(x)$ to s_7, if we choose $N = 4$ and $M = 3$ we arrive at the set of equations

$$\begin{aligned}
a_0 &= s_0 \\
a_1 &= b_1 s_0 + s_1 \\
a_2 &= b_2 s_0 + b_1 s_1 + s_2 \\
a_3 &= b_3 s_0 + b_2 s_1 + b_1 s_2 + s_3 \\
a_4 &= b_3 s_1 + b_2 s_2 + b_1 s_3 + s_4 \\
a_5 = 0 &= b_3 s_2 + b_2 s_3 + b_1 s_4 + s_5 \\
a_6 = 0 &= b_3 s_3 + b_2 s_4 + b_1 s_5 + s_6 \\
a_7 = 0 &= b_3 s_4 + b_2 s_5 + b_1 s_6 + s_7 \\
a_8 = 0 &= b_3 s_5 + b_2 s_6 + b_1 s_7 + s_8 \qquad (2.5)
\end{aligned}$$

where the first 8 lines allow us to determine the unknown coefficients of the Padé Approximant and the last line, perhaps the most important, allows us to approximate the coefficient of the next term in the series $S(x)$ which was, until now, unknown. This term, s_8 in this case, is called the Padé Approximant Prediction (PAP).

2.1 Examples of the PA and PAP

To make the method of the Padé Approximants clearer, and to demonstrate their power in making predictions and converging to the formal sum faster than the partial sums, I will now give two concrete examples of well-known functions. The power of this method is seldom appreciated fully until it is seen in action, and I believe these examples will serve to convince the reader that this is, in fact, a most useful tool.

2.1.1 The [4/3] PA and PAP to $\frac{\ln(1+x)}{x}$ at $x = 1$

To show the power of the Padé Approximant, let us choose the function to be

$$\frac{\ln(1+x)}{x} = 1 - \frac{1}{2}x + \frac{1}{3}x^2 - \frac{1}{4}x^3 = \cdots$$

and again choose the [4/3] Padé . The simultaneous equations can be expressed in matrix form as

$$\mathbf{B}\cdot\mathbf{S}=\mathbf{A} \tag{2.6a}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_2 & b_1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_3 & b_2 & b_1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_3 & b_2 & b_1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3 & b_2 & b_1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_3 & b_2 & b_1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_3 & b_2 & b_1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_3 & b_2 & b_1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -\frac{1}{2} \\ \frac{1}{3} \\ -\frac{1}{4} \\ \frac{1}{5} \\ -\frac{1}{6} \\ \frac{1}{7} \\ -\frac{1}{8} \\ s_8 \end{pmatrix} = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.6b}$$

which can be solved uniquely since the matrix $\mathbf{B}$ is nonsingular *. Putting this equation into *Mathematica* we find the solutions

$$\begin{aligned} a_0 &= 1 \\ a_1 &= \frac{11}{8} \\ a_2 &= \frac{157}{336} \\ a_3 &= \frac{1}{56} \\ a_4 &= -\frac{1}{1120} \\ b_1 &= \frac{1}{15} \\ b_2 &= \frac{15}{14} \\ b_3 &= \frac{5}{28} \end{aligned} \tag{2.7}$$

*Note that since the matrix is upper triangular, the determinant is trivially unity.

The predicted value of s_8 is 0.111076 to be compared to the actual value of $1/9 = 0.111111$. Also of note is that the $[N/M]$ Padé Approximant is a more accurate value than the partial sum of the same order. For this example, $[4/3]_{(x=1)} = 0.693146$ to be compared to the actual value of $\ln 2 = 0.693147$ and the partial sum to order 7, 0.634524.

2.1.2 The [4/3] PA and PAP to e^x at $x = 1$

We now take the series to be

$$e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots \tag{2.8}$$

and assume that only the first several terms are known. Again using the [4/3] Padé Approximant we have the same matrices **A** and **B** while **S** has changed.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_2 & b_1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_3 & b_2 & b_1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_3 & b_2 & b_1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3 & b_2 & b_1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_3 & b_2 & b_1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_3 & b_2 & b_1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_3 & b_2 & b_1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ \frac{1}{2!} \\ \frac{1}{3!} \\ \frac{1}{4!} \\ \frac{1}{5!} \\ \frac{1}{6!} \\ \frac{1}{7!} \\ s_8 \end{pmatrix} = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.9}$$

Again using *Mathematica* we find the solutions

$$\begin{aligned} a_0 &= 1 \\ a_1 &= \frac{4}{7} \\ a_2 &= \frac{1}{7} \\ a_3 &= \frac{2}{105} \\ a_4 &= \frac{1}{840} \\ b_1 &= -\frac{3}{7} \\ b_2 &= \frac{1}{14} \\ b_3 &= -\frac{1}{210} \end{aligned} \tag{2.10}$$

The Padé Approximant Prediction of s_8 is 2.55102×10^{-5} while the exact value is $\frac{1}{81} = \frac{1}{40320} = 2.48015 \times 10^{-5}$. The Padé Approximant is

$$\frac{1 + \frac{4}{7} + \frac{1}{7} + \frac{2}{105} + \frac{1}{840}}{1 - \frac{3}{7} + \frac{1}{14} - \frac{1}{210}} = 2.718283582 \tag{2.11a}$$

while the partial sum is

$$1 + 1 + \frac{1}{2!} + \frac{1}{3!} + \frac{1}{4!} + \frac{1}{5!} + \frac{1}{6!} + \frac{1}{7!} = 2.718253968 \tag{2.11b}$$

both of which should be compared to the exact value

$$e^1 = 2.718281728 \tag{2.11c}$$

It is theoretically possible to extend this method to higher orders by using the predicted results as input for the next calculation. However, as I discuss later, this method introduces unpredictable and compounding errors.

CHAPTER 3

4- and 5-Loop Predictions

3.1 A Brief Introduction to Quantum Field Theories

In Quantum Field Theories, the β function is given by the relation

$$\beta(g) = \mu \frac{\partial g}{\partial \mu} \tag{3.1}$$

where μ is the energy scale of the interaction and g is the coupling "constant". In the ϕ^4 theory the coupling is given the symbol "λ", in QED it is "e", and in QCD we use "g_s". In this paper I will use the more common QCD parameter $\alpha_s = g_s^2/4\pi$. It is also notable that while the β function is itself a polynomial in the coupling constant, each of the coefficients is also a polynomial. In QCD these coefficients are polynomials in the number of quark flavors taking place in the interaction, N_F. So the QCD β-Function can be written as

$$\begin{aligned} \beta(\alpha_s) &= -\beta_0 \frac{\alpha_s}{\pi} - \beta_1 \left(\frac{\alpha_s}{\pi}\right)^2 - \beta_2 \left(\frac{\alpha_s}{\pi}\right)^3 + O(\alpha_s^4) \\ &= -\{A_0 + B_0 N_F\} \frac{\alpha_s}{\pi} - \{A_1 + B_1 N_F\} \left(\frac{\alpha_s}{\pi}\right)^2 \\ &\quad -\{A_2 + B_2 N_F + C_2 N_F^2\} \left(\frac{\alpha_s}{\pi}\right)^3 + O(\alpha_s^4) \end{aligned} \tag{3.2}$$

3.2 The WAPAP at Order 4-Loops

It has been shown [8,3] that if the coefficients of a series, S_n, diverge as $n!$ for large n, then the relative error of the PAP is given by

$$\varepsilon_{N+M+1} = \frac{S^{PAP}_{N+M+1} - S_{N+M+1}}{S_{N+M+1}} \tag{3.3}$$

and that for a fixed value of M

$$\lim_{N\to\infty} \varepsilon_{N+M+1} = -\frac{M! A^M}{L^M_{[N/M]}} \tag{3.4}$$

where $L_{[N/M]} = N + M + aM + b$, with A, a, b constant. We greatly simplify the prediction by only considering the cases where $M = 1$. With this prescription we have the means to correct the asymptotic behavior of the PAP, thus resulting in the Asymptotic Padé Approximant Prediction (APAP)

$$S^{APAP}_{N+M+1} \equiv \frac{S^{PAP}_{N+M+1}}{1 + \epsilon_{N+M+1}} \tag{3.5}$$

It has been noted that we can now make a further refinement of our method by using a weighting procedure over the values used in the χ^2 fit of S^{APAP}_{N+M+1}. Since the β-function can be written as a polynomial in the number of quark flavors involved in the process, *i.e.* $\beta_j = A_i + B_i N_F + C_i N_F^2 + \cdots + X_i N_F^i$, we can find the Padé Approximant over a range of values of N_F. It has been observed that more accurate predictions are found, in most cases, if the fit is done over *negative* values of N_F. While this may initially strike us as a problem with the method, we must remember that while the β-function is representative of a physical quantity, the APAP method is simply a mathematical tool and is thus not restricted to the physical realm $N_F > 0$. The introduction of a rational function to approximate a polynomial clearly creates the possibility of vertical asymptotes in the $\beta - N_F$ plane. This is, in fact, the case in QCD where the prediction β_3^{APAP} has vertical asymptotes at $N_F \in \{6.2228, 8.05263, 12.4095, 84.3174\}$. It is these vertical asymptotes at positive values of N_F which prompts us to use negative values for the χ^2 fit.

My method of calculation is based on algebraically manipulating the input functions and then evaluating them over the various N_F (App. B). This method allows not only the answers to the question of using negative N_F, but makes it very easy to perform the method on any interval we wish rather than just working on integer values. We can now argue that because the predicted values are the result of a χ^2 fit, the most accurate values of the coefficients of the polynomial form of the β function are given when the coefficient times the corresponding power of N_F is equal

to the constant term. *i.e.*

$$\begin{aligned} A_j &= B_j \frac{1}{N_F^{max}+1} \sum_0^{N_F^{max}} N_F = \frac{B_j N_F^{max}}{2} \equiv B_j^W \\ A_j &= C_j \frac{1}{N_F^{max}+1} \sum_0^{N_F^{max}} N_F^2 = \frac{C_j N_F^{max}(2N_F^{max}+1)}{6} \equiv C_j^W \\ &\vdots \quad \vdots \end{aligned} \tag{3.6}$$

In most respects, my method of weighting mirrors that of reference [1] except for the "interpolation" factor. For two consecutive values of B, call them $B^{(1)}$ and $B^{(2)}$, and the corresponding N_F I calculate the predicted value, call it $B^{(p)}$ by

$$B^{(p)} = B^{(1)} \frac{B^{(1)} N_F^{(1)} + B^{(2)} N_F^{(2)}}{B^{(1)} N_F^{(2)} + B^{(2)} N_F^{(1)}} \tag{3.7}$$

This new method, as used by the authors of [1], is called the Weighted Asymptotic Padé Approximant Predictions (WAPAP). Eventhough I have used a different method in my calculations, I will also use this nomenclature when I refer to my results.

3.2.1 The QCD β-Function

The QCD β function up to and including the three-loop level in MS-type schemes is

$$\beta(\alpha_s) = -\beta_0 \frac{\alpha_s}{\pi} - \beta_1 \left(\frac{\alpha_s}{\pi}\right)^2 - \beta_2 \left(\frac{\alpha_s}{\pi}\right)^3 + O(\alpha_s^4) \tag{3.8}$$

And each of the coefficients β_i are themselves polynomials in the number of quark flavors involved in the process, N_F, and other representation-group-dependent factors. The expressions C_A, C_F and T are group operators dependent on the symmetry group of the theory. (App. A)

$$\begin{aligned} \beta_0 &= \frac{1}{4}\left(\frac{11}{3}C_A - \frac{4}{3}TN_F\right) \\ \beta_1 &= \frac{1}{16}\left(\frac{34}{3}C_A^2 - \frac{20}{3}C_A T N_F - 4C_A T N_F\right) \\ \beta_2 &= \frac{1}{64}\left(\frac{2857}{54}C_A^3 - \frac{1415}{27}C_A^2 T N_F + \frac{158}{27}C_A T^2 N_F^2 \right. \\ &\quad \left. - \frac{205}{9}C_A C_F T N_F + \frac{44}{9}C_F T^2 N_F^2 + 2C_F^2 T N_F\right) \end{aligned} \tag{3.9}$$

The β function coefficient at four loops is given by,

$$\begin{aligned}
\beta_3 &= \left\{ C_A^4 \left(\frac{150653}{486} - \frac{44}{9}\zeta_3 \right) + C_A^3 T_F N_F \left(-\frac{39143}{81} + \frac{136}{3}\zeta_3 \right) \right. \\
&+ C_A^2 C_F T_F N_F \left(\frac{7037}{243} - \frac{656}{9}\zeta_3 \right) + C_A C_F^2 T_F N_F \left(-\frac{4204}{27} + \frac{352}{9}\zeta_3 \right) \\
&+ 46 C_F^3 T_F N_F + C_A^2 T_F^2 N_F^2 \left(\frac{7930}{81} + \frac{224}{9}\zeta_3 \right) + C_F^2 T_F^2 N_F^2 \left(\frac{1352}{27} - \frac{704}{9}\zeta_3 \right) \\
&+ C_A C_F T_F^2 N_F^2 \left(\frac{17152}{243} + \frac{448}{9}\zeta_3 \right) + \frac{424}{243} C_A T_F^3 N_F^3 + \frac{1232}{243} C_F T_F^3 N_F^3 \\
&+ \frac{d_A^{abcd} d_A^{abcd}}{N_A} \left(-\frac{80}{9} + \frac{704}{3}\zeta_3 \right) + N_F \frac{d_F^{abcd} d_A^{abcd}}{N_A} \left(\frac{512}{9} - \frac{1664}{3}\zeta_3 \right) \\
&+ \left. N_F^2 \frac{d_F^{abcd} d_F^{abcd}}{N_A} \left(-\frac{704}{9} + \frac{512}{3}\zeta_3 \right) \right\} \qquad (3.10)
\end{aligned}$$

This can be put into the usual form by collecting powers of N_F and using the simple expression

$$\beta_3 = A_3 + B_3 N_F + C_3 N_F^2 + D_3 N_F^3 \qquad (3.11)$$

It is these values of A_3, B_3, and C_3 that I have predicted using the Padé method. The values I have computed are shown in Table 3.2.1, along with the exact results [9] and those of John Ellis, Ian Jack, Tim Jones, Marik Karliner, and Mark Samuel [2].

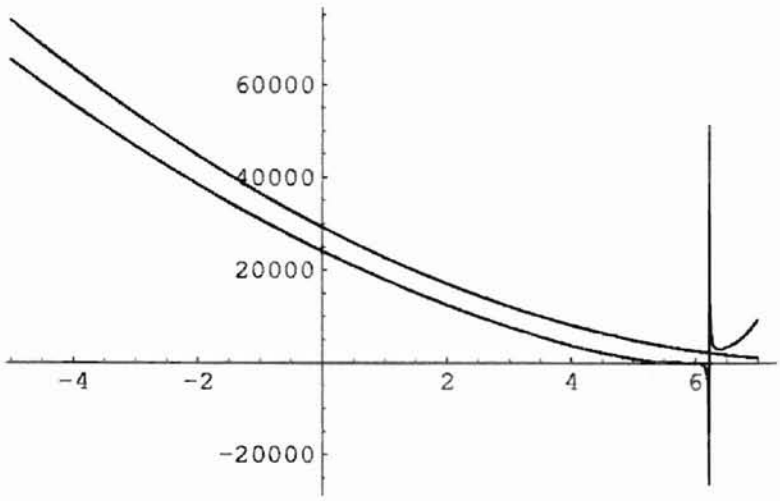

Figure 3.1. The APAP for the QCD β-Function Coefficient plotted vs. the actual β-Function at order 4-loops in the $N_F - \beta_3$ plane. Note the vertical asymptote in the APAP graph which forces us to use $N_F^{max} < 0$. Other values of N_F for which the denominator of our APAP is zero are all positive.

	JFH	$EJJKS$	$EXACT$	$\%error(JFH)$	$\%error(EJJKS)$
A_3	24625.2	24670	24632.8	−0.03086	0.13
B_3	−6371.7	−6383	−6374.55	−0.04471	0.13
C_3	402.7665	405	398.478	1.07622	1.6
D_4	*input*	*input*	1.49931	− − − − −	− − − − −

TABLE 3.1. The QCD β-Function at 4-Loops with N_F=3 and N_c=3. Current predictions (JFH) vs. those of Ellis, Jack, Jones, Karliner, and Samuel (EJJKS) and the exact values (EXACT). Percent errors are also given for both methods of prediction. The value for D_4 was input from large N_F calculations [4].

3.2.2 Other 4-Loop Predictions

I have applied this method to other series from QFT's and while the results are, in some cases, not as impressive as those found in QCD, the method still seems to be a reliable predictor of the perturbative coefficients.

Of particular note are the results for the scalar ϕ^4 theory since it is known exactly at 5, and higher, loops. The ϕ^4 theory is characterized by the Lagrangian

$$\mathcal{L} = \frac{1}{2}\left(\partial_\mu \phi_0\right)^2 - m_0^2\phi_0^2 - \frac{1}{4!}\lambda_0\phi_0^4 \tag{3.12}$$

Notice especially that the errors in QCD are much smaller than the errors of the predictions for ϕ^4. I believe that this will also be true at the 5-loop level, and that the predicted error in ϕ^4 sets a strict, and generous, upper bound on the error.

The most disquieting results are those for Supersymmetric Quantum Chromodynamics (SQCD) in the NSVZ renormalization scheme [7,5,6]. This scheme is proported to be an exact theory, yet the error of the Padé is significant in this case. Dr. Ellis has conjectured that perhaps the Padé method is sensitive to the Minimal Subtraction (MS or $\bar{M}S$) schemes, since it is guided by the ϕ^4 theory, and that this could be the reason the NSVZ scheme does not yield accurate values. It should be noted that the correct values for the NSVZ scheme are included in the generated predictions, it is only that the weighting does not select those values in this case.

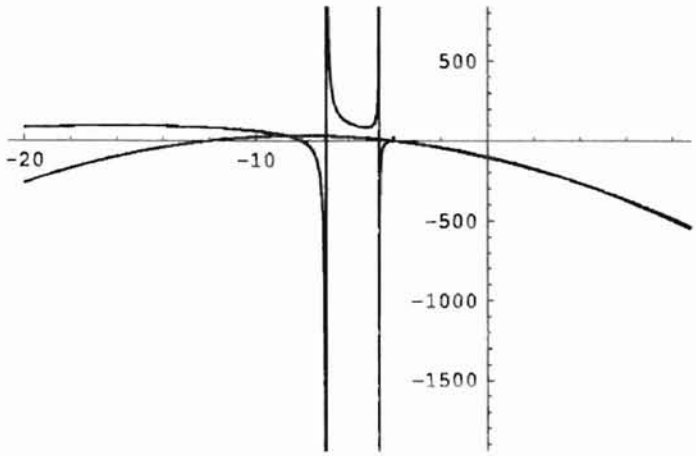

Figure 3.2. The APAP for the ϕ^4 β-Function Coefficient plotted vs. the actual β-Function Coefficient at order 4-loops in the $N_F - \beta_3$ plane. Note that the vertical asymptote in this case occurs at *negative* N_F, thus we use $N_F^{max} > 0$ for the χ^2 fit.

	JFH	*EXACT*	*%error*
A_3	-105.12	-100.463	4.636
B_3	-34.21	-33.281	2.7925
C_3	-1.8800	-2.0593	-8.705
D_4	*input*	0.000643	– – – – –

TABLE 3.2. The ϕ^4 β-Function at order 4-Loops.

	JFH	*EXACT*	*%error*
A_3	-7807.59	-7776	0.4063
B_3	3094.753	3207.19	-3.508
C_3	-515.082	-451.626	14.051
D_4	*input*	$-.222222$	– – – – –

TABLE 3.3. The SQCD β-Function in the DRED scheme at order 4-Loops.

	JFH	*EXACT*	*%error*
A_3	-2044.24	-1944	5.15633
B_3	682.8961	990.519	-31.0567
C_3	-158.584	-231.331	-31.4471
D_4	*input*	-5.33333	– – – – –

TABLE 3.4. The SQCD β-Function in the NSVZ scheme at order 4-Loops.

	JFH	*EXACT*	*%error*
A_3	96.44787	96.4386	0.00961
B_3	-21.0668	-18.8291	11.884
C_3	0.299205	0.276163	8.3436
D_4	*input*	0.00579	– – – – –

TABLE 3.5. The Anomalous Quark Mass Dimension

3.3 The WAPAP at Order 5-Loops.

We again start with the standard PAP

$$\beta_4^{PAP} = \frac{\beta_3^2}{\beta_2} \tag{3.13}$$

and compute the errors in the same manner as the 4-Loop case. It should be noted that my method differs from that of [1] in that I do not calculate $\mathcal{A}$ and a+b but do the entire calculation by algebraically manipulating the lower-order, known terms of the series. (App. B)

In the exact calculation [3] of the 4-Loop QCD β-Function there occurred, for the first time, quartic Casimir operators. Since the PAP uses the earlier terms to estimate the first unknown, the contributions due to these non-planar diagrams could not be predicted. It was assumed, and later verified by the exact calculation, that the contributions from a new *type* of diagram should be very small compared to the evolution of the already existing types. We assume that the same will hold true in the 5-Loop orders, and that our prediction will thus be a good, though not perfect, estimation.

Without the exact values of these functions at order 5-Loop, how are we to know if our predictions are even reasonable? I offer two suggestions based on our freedom to do the χ^2 fit of the data with either the known value of E_4 input or leave E_4 as a free parameter to be determined in the fit.

- If we leave E_4 free, we can then compare it to the known value
- We can consider the stability of all the coefficients comparing the two different fitting schemes. A small change might instill confidence, while a large change in any of the coefficients could undermine our confidence in the results.

Of particular importance is the accuracy of the highest-order term when it is left as a free parameter. It is seen that in almost all cases under consideration, the highest-order term is approximately 5 orders of magnitude smaller, 1/10000, than the lowest-order (constant) term. The accuracy of this parameter then gives a very finely

tuned estimate of the accuracy of the fit; especially when one considers that for the smaller values of N_F, this term is negligible when compared to the constant, but for $N_F >\approx 12$ this term dominates all others in the polynomial.

A final check of the accuracy of the prediction might be to compare the constant term in the WAPAP fit to an average of the values of the functions from the χ^2 fit at $N_F = 0$. Since I have generated 20 or more predictions of the β function, as $N_F = N_F^{min} \rightarrow N_F^{max}$, I will have a large number of predicted values of A_n which I can compare the prediction with. For example, in the QCD case at 4-Loops, I used $|N_F^{min}| = 2$ and $|N_F^{max}| = 20$. Thus I can evaluate each of these 19 functions at $N_F = 0$ and average the results; doing this I find $\bar{A}_3 = 24891.45$, very close to the WAPAP $A_3 = 24625.2$ and the exact result $A_3 = 24632.8$. The standard deviation at order 4-Loop is 696.85, or less than 2%. Similarly for the 5-Loop predictions, without the quartic Casimir contributions, we find that in the cases of holding E_4 fixed, $\bar{A}_4 = 470886$ to be compared to the WAPAP $A_4 = 471307$; the standard deviation is 2983, or 0.6%. In the case of allowing E_4 to be a free parameter, $\bar{A}_4 = 468295$ while the WAPAP is $A_4 = 468500$; the standard deviation is 2076.7, or .44%.

While none of these criterion is, in and of itself, a guarantee of the prediction's correctness, the high degree of correlation amongst all of them does tend to make the prediction more credible. Of course, the true accuracy of these predictions may never be known. The exact calculation of β_4 is a daunting task which almost certainly could not be completed in less than several decades given current calculation techniques.

	$E-fixed, wC$	$E-free, wC$	$\%diff$
$A_4(JFH)$	720013.9	719459	0.0771
$A_4(EJJKS)$	759000	751000	1.06
$B_4(JFH)$	−210918.2	−211473.6	−0.263
$B_4(EJJKS)$	−219000	−220000	−0.456
$C_4(JFH)$	19583.32	18856.02	3.78
$C_4(EJJKS)$	20500	19700	3.98
$D_4(JFH)$	−52.486	−65.689	−22.3
$D_4(EJJKS)$	−49.8	−93.8	−61.3
$E_4(JFH)$	−1.84	−1.874	−1.83
$E_4(EJJKS)$	−1.84	−2.03	−9.82

TABLE 3.6. The QCD β-Function at Order 5-Loop with the 4-Loop Quartic Casimir contributions. The two treatments of E_4 are shown as E-fixed and E-free. Percent differences are then shown to give a measure of stability.

	$E-fixed, w/oC$	$E-free, w/oC$	$\%diff$
$A_4(JFH)$	471307.5	468500.6	0.597
$A_4(EJJKS)$	488000	485000	0.617
$B_4(JFH)$	−151088	−151446	−0.237
$B_4(EJJKS)$	−156000	−157000	−0.640
$C_4(JFH)$	15779.96	15258.83	3.36
$C_4(EJJKS)$	16400	15800	3.73
$D_4(JFH)$	−61.849	−147.047	−81.6
$D_4(EJJKS)$	−60.5	−163	−91.7
$E_4(JFH)$	−1.84	−2.339	−23.8
$E_4(EJJKS)$	−1.84	−2.56	−32.7

TABLE 3.7. The QCD β-Function at Order 5-Loop Without the Quartic Casimir contributions. The two treatments of E_4 are shown as E-fixed and E-free. Percent differences are then shown to give a measure of stability.

	Predicted	*EXACT*	*%error*
$A_4(JFH)$	954.1259	1001.99	−4.777
$B_4(JFH)$	366.6934	385.604	−4.904
$C_4(JFH)$	37.33699	30.2681	23.352
$D_4(JFH)$	0.319645	0.576413	−44.546
$E_4(JFH)$	*input*	−0.00129	− − −−

TABLE 3.8. The $\phi^4\beta$-Function at Order 5-Loop. Percent errors are also shown.

	$E-fixed$	$E-free$	$\%diff$
$A_4(JFH)$	118402	118413	−0.00929
$A_4(EJJKS)$	113000	112000	0.889
$B_4(JFH)$	−61057.05	−61294.33	−0.388
$B_4(EJJKS)$	−58500	−58700	−0.341
$C_4(JFH)$	13206.9	12810.4	3.04
$C_4(EJJKS)$	12900	12500	3.15
$D_4(JFH)$	−301.75	−374.54	−12.5
$D_4(EJJKS)$	−307	−400	−26.3
$E_4(JFH)$	−6.64	−3.814	54.1
$E_4(EJJKS)$	−6.64	−4.53	37.8

TABLE 3.9. The SQCD β-Function in the DRED Scheme at Order 5-Loop. The two treatments of E_4 are shown as E-fixed and E-free. Percent differences are then shown to give a measure of stability.

	$E-fixed$	$E-free$	$\%diff$
$A_4(JFH)$	10974	16169.11	−38.28
$A_4(EJJKS)$	10400	10500	−0.957
$B_4(JFH)$	−1970.202	−1315.32	39.86
$B_4(EJJKS)$	−7870	−7800	0.8934
$C_4(JFH)$	3297.47	2953.597	11.00
$C_4(EJJKS)$	3100	2870	7.705
$D_4(JFH)$	−109.7583	−134.719	−20.419
$D_4(EJJKS)$	−90.1	−241	−91.151
$E_4(JFH)$	−7.49	−7.04659	6.101
$E_4(EJJKS)$	−7.49	−13.28	−55.753

TABLE 3.10. The SQCD β-Function in the NSVZ Scheme at Order 5-Loop. The two treatments of E_4 are shown as E-fixed and E-free. Percent differences are then shown to give a measure of stability.

CHAPTER 4

Error Estimates for the 4- and 5-Loop β-Functions

4.1 Method for Estimating Error

Because the Padé Approximant is closely related to the Taylor expansion of a function, notice that the $[N/0]$ PA is identically the N^{th} order Taylor series, we know that the errors of the Approximants must satisfy

$$\lim_{N\to\infty} \epsilon = 0 \; \forall M. \tag{4.1}$$

It is unfortunate, however, that the behavior of the error at small N is not predictable. For example, the error for the function $\frac{\ln(x+1)}{x}$ in the [4/3] PAP is 0.03088%, while at the next order we have the error in the $[4/4] = 0.0063\%$ and in the [5/3] the error is 0.01417%. In the case of e^x, the errors are $\epsilon([4/3]) = 2.857$, $\epsilon([4/4]) = 1.42857$, and $\epsilon([5/3]) = 1.78571$. So although the error is reduced with more input, the reduction is not predictable either as an absolute amount or percentage. Thus it is necessary to derive an alternative method to predict the error.

Recall that at order 4-loops, the coefficient of the β function is a polynomial which can be written

$$\beta_3 = A_3 + B_3 N_F + C_3 N_F^2 + D_3 N_F^3 \tag{4.2}$$

It is in the case of estimating errors that the previously undesireable aspect of the coefficients of the β function being themselves polynomials becomes an asset. Since a χ^2 fit over progressivly longer intervals was performed to find these polynomials, I have generated from twenty, at order 4-loops, to forty, at order 5-loops, values of each term in the polynomial. Thus I can consider that, for example, at order 4-loops I have a polynomial representation of the constant term A and the value chosen, 24625.2,

is simply a point on that curve. For example, in regular QCD at order 4-loops, the data are

N_F^{max}	A	B	C
-2	24137.3	-6447.86	331.999
-3	24168.1	-6448.46	336.528
-4	24201.5	-6444.25	341.697
-5	24239.4	-6434.88	347.365
$\vdots$	$\vdots$	$\vdots$	$\vdots$
-20	26445.3	-5582.54	457.276

TABLE 4.1. Predictions generated for the A, B and C curves as N_F^{max} ranges from -2 to -20.

I can now perform a χ^2 fit of these data points to find A_3, B_3, and/or C_3 independently as a function of N_F^{max}. I can then perform any number of evaluations on them, including finding radius of curvature, extremum, etc. It is, in fact, the radii of curvature that finally led to a means by which the error of the WAPAP's can be predicted.

As is usually the case, the method grew out of trial and error on the ϕ^4 theory. This scalar QFT was used as a guide because it is known to order 5-loops and thus enables us to examine the development of the WAPAP's as the order is increased. Taking the data generated by the WAPAP process, I fit the coefficients A, B, and C to cubic polynomials,

$$\begin{aligned} A(N_F) &= -105 + 0.281N_F - 0.0263N_F^2 + 1.73 \times 10^{-4}N_F^3 \qquad (4.3) \\ B(N_F) &= -34.7 + 0.0667N_F + 8.17 \times 10^{-4}N_F^2 + 4.03 \times 10^{-4}N_F^3 \\ C(N_F) &= -1.6 - 0.00822N_F - 0.00175N_F^2 + 7.11 \times 10^{-5}N_F^3 \end{aligned}$$

for which I found the raduis of curvature at the N_F' corresponding to the value $B^{(p)}$ *. I then calculate two values, d and d' which are the orthogonal distance from the point $(N_F', B^{(p)})$ to the curve and the vertical distance from $(N_F', B^{(p)})$ to the curve, respectively. These values I then divided by $B^{(p)}$ and called the results ϵ and ϵ'.

The values ϵ and ϵ' can thus be thought of as a percent measurement of the error between the value predicted by the interpolation of equation 3.7 and the χ^2 fit of the data. There are at least two natural questions to ask at this point, and I now present them with answers.

1. Why fit the data to a cubic polynomial as opposed to a quadratic, quartic or quintic?

    - In doing the χ^2 fits of the data, the coefficients changed drastically in going from a quadratic to a cubic polynomial, but there was little, if any, change in going from fitting a cubic to a quartic polynomial. The coefficient of the new term, N_F^4, was at least four orders of magnitude smaller than the N_F^3 coefficient, and the other coefficients changed by less than 0.001%.

2. Can the ϵ and/or ϵ' be related to the errors in the WAPAP?

    - Yes, the value ϵ' seems to very closely related to the error of the WAPAP. This correlation is best in MS-type regularization schemes, and is not as good in other types.

*All the curves were single-valued around this point, hence inverting to find N_F' was a trivial exercise

4.2 Error Bars at Order 4-Loop

Once the data points are fit to a polynomial, the radius of curvature is given by the formula

$$R(N_F) = \frac{|d^2y/d^2N_F|}{(1+(d^2y/d^2N_F)^2)^{3/2}} \tag{4.4}$$

where y is any of the polynomials A, B, or C. I then evaluate the raduis of curvature and the value of the polynomial at the value of N'_F which corresponds to $B^{(p)}$. From this I calculate the value of ϵ' to be

$$\epsilon' = \sqrt{\left|\frac{R(N'_F) - R(N'_F)\sqrt{1-\frac{1}{4(R(N'_F))^2}}}{y(N'_F)}\right|} \tag{4.5}$$

and define the 4-loop Error Parameter, σ, to be

$$\sigma \equiv \left\lfloor \frac{\epsilon^{WAPAP}}{\epsilon'} \right\rfloor \tag{4.6}$$

For ϕ^4 the values ϵ' for the A, B and C curves are, $\epsilon'_A = .876871$, $\epsilon'_B = .702197$ and $\epsilon'_C = .423359$ while the actual errors of the Padé approximant are 4.6355, 2.9726 and -8.70482, respectively. Thus the 4-loop Error Parameters are

$$\sigma_A = 6$$

$$\sigma_B = 4$$

$$\sigma_C = 21$$

For QCD, $N_F = 3$, the ϵ', $\sigma\epsilon'$ and actual error are shown in table 4.2. As you can see this method gives quite generous error estimates for QCD. Unfortunately, that is not the case with other theories. Again, perhaps supporting the hypothesis of John Ellis that Padé , at least a Padé scheme based on the ϕ^4 theory, doesn't like non-minimal subtraction schemes, the DRED formalism works fairly well while the NSVZ results are less than adequate.

	ϵ'	$\sigma\epsilon'$	%error
A	.884354	5.306	−0.03086
B	.190030	0.7601	−0.04471
C	.18712	3.930	1.07622

TABLE 4.2. The 4-Loop for Error Estimate for the Quantum Chromodynamics β function.

	ϵ'	$\sigma\epsilon'$	%error
A	.1990625	1.194	0.406313
B	1.61415	6.457	−3.50578
C	.793347	16.66	14.051

TABLE 4.3. The 4-Loop Error Estimate for SQCD in the DRED scheme

	ϵ'	$\sigma\epsilon'$	%error
A	2.75147	16.51	5.0948
B	4.10948	16.438	−31.0567
C	.83844	17.61	−32.2457

TABLE 4.4. The 4-Loop Error Estimate for SQCD in the NSVZ scheme

4.3 Error Bars at Order 5-Loop

Again we look initially to the ϕ^4 theory to give us the value of the 5-loop Error Parameter. This is then applied to the Padé Approximant Prediction of the 5-Loop coefficient with the 4-Loop Quartic Casimir operators included in the calculation. It is my conclusion that these predictions are validated by the small percent errors derived from this method in addition to the confidence gained by such factors as the stability of the prediction as E_4 is either included in or set before the calculation.

	ϵ'	%error	σ
A	1.1476	−4.77691	5
B	0.91332	−4.90415	6
C	1.12076	23.35424	21
D	1.55061	−44.5458	29

TABLE 4.5. The Error Parameter from 5-loop ϕ^4

	ϵ'	$\sigma\epsilon'$	estimated coefficient
A	0.446621	2.2331	720013.9 ± 16078.6
B	0.797506	4.78684	-210918 ± 10096.3
C	0.103368	2.17073	19583.32 ± 425.101
D	0.13042	3.78210	-52.4863 ± 1.9851

TABLE 4.6. The Error Estimate for 5-loop QCD with contributions from 4-Loop Quartic Casimir Operators

CHAPTER 5

Summary and Conclusions

5.1 Summary

I have introduced the Padé Approximant Prediction (PAP) and the refinements which give rise to the Weighted Asymptotic Padé Approximant Prediction (WAPAP). Through the demonstration of this method using both well known mathematical series, e_x and $\log(1+x)/x$, and known series from Quantum Field Theories I have shown that this is indeed a reliable and accurate predictive tool. Plausible arguments were then made for methods of controlling and estimating errors. A particular method was then introduced and shown to work well at the 4-Loop order for QFT's utilizing the $\bar{M}S$ renormalization method.

The techniques shown to be reliable at order 4-Loops were then applied to series at order 5-Loops.

5.2 Conclusions

While the exact 5-Loop coefficient of the considered series is only known for the scalar ϕ^4 theory, the reliability and accuracy of the 4-Loop calculations is very likely reproduced. As evidence of this is my "Error Parameter" method which was shown to give reliable and even generous error bars at the 4-Loop order and was less than 5% for all coefficients at 5-Loops.

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APPENDICES

APPENDIX A

Symbols and Notation

N_F	The number of quark flavors involved in an interaction
C_A	The number of quark colors, taken to be 3
C_F	$\frac{1}{C_A^2-1}$
T	An $SU(N)$ Operator, by convention $T = 1/2$ in $SU(3)$.
ζ_3	The Reimann Zeta Function evaluated at 3. Approximately 1.2020569
ε_{N+M+1}	The Asymptotic Error of the Predictions

APPENDIX B

Mathematica Code Used to Calculate β functions

For the sake of clarity, I include and example of the code used to generate the predictions. This is the calculation of the 4-loop β function in QCD. I have only included output from *Mathematica* where it seems necessary.

We begin by giving a numeric approximation to the Reimann Zeta Function, setting the Quartic Casimir Operators to 0 and entering the first three coefficients of the β function.

$$\zeta = 1.2020569$$

$$d_A^{abcd} d_A^{abcd} = 0$$

$$d_F^{abcd} d_F^{abcd} = 0$$

$$d_F^{abcd} d_A^{abcd} = 0$$

$$\begin{aligned}
\beta_0 &= \frac{1}{4}\left(\frac{11}{3}C_A - \frac{4}{3}TN_F\right) \\
\beta_1 &= \frac{1}{16}\left(\frac{34}{3}C_A^2 - \frac{20}{3}C_A T N_F - 4C_A T N_F\right) \\
\beta_2 &= \frac{1}{64}\left(\frac{2857}{54}C_A^3 - \frac{1415}{27}C_A^2 T N_F + \frac{158}{27}C_A T^2 N_F^2\right. \\
&\quad \left. -\frac{205}{9}C_A C_F T N_F + \frac{44}{9}C_F T^2 N_F^2 + 2C_F^2 T N_F\right)
\end{aligned} \tag{B.1}$$

The Padé Approximant to β_2 is then given by

$$\begin{aligned}
PAP_{\beta_2} &= \frac{(\beta_1)^2}{\beta_0} \\
&= \frac{(\frac{34}{3}N_C^2 - (\frac{10}{3}N_C + \frac{N_C^2-1}{N_C})N_F)^2}{\frac{11}{3}N_C - \frac{2}{3}N_F}
\end{aligned}$$

from which we calculate the asymptotic error formula

$$R = \frac{1}{2}\frac{PAP_{\beta_2} - \beta_2}{\beta_2} \tag{B.2}$$

$$= \frac{-21238N_C^6+3N_C(-99+391N_C^2+5734N_C^4)N_F-6(-63+160N_C^2+536N_C^4)N_F^2+4N_C(-33+112N_C^2)N_F^3}{2(11N_C-2N_F)(5714N_C^5-(-27-561N_C^2+3418N_C^4)N_F+2N_C(-33+112N_C^2)N_F^2)}$$

We now construct the Padé Approximant for for the 4-loop coefficient

$$PAP_{\beta_3} = \frac{(\beta_2)^2}{\beta_1} \tag{B.3}$$

and including the asymptotic error formula we arrive at the Asymptotic Padé Approximant Prediction (APAP) at 4-loops,

$$APAP_{\beta_3} = \frac{PAP_{\beta_3}}{1+R} \tag{B.4}$$

$$= \frac{-(-11N_C+2N_F)(5714N_C^5+(27+561N_C^2-3418N_C^4)N_F+2N_C(-33+112N_C^2)N_F^2)^3}{1944N_C^5(84N_C^3+8N_F-18N_C^2N_F)(104470N_C^9+(297N_C+18515N_C^3-80850N_C^5)N_F+6(45-776N_C^2+2564N_C^4)N_F^2+(182N_C-448N_C^3)N_F^3)}$$

which at $N_C = 3$ is given by

$$\frac{-\left((-33+2N_F)\left(1388502-271782\,N_F+5850N_F^2\right)^3\right)}{52488(918-114N_F)\left(6158630-19280754N_F+1204470N_F^2-11700N_F^3\right)}$$

This APAP is then fit to a second degree polynomial over the intervals $N_F \in \{0, N_F^{max}\}$ as $|N_F^{max}| = 2, 3, 4, ...20$ yielding predictions for A_3, B_3 and C_3 at each value of N_F. It is these values which are then entered into the "weighting" process.

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