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Estimating Perturbative Coefficients in Quantum Field Theory and Statistical Physics

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We present a method for estimating perturbative coefficients in quantum field theory and statistical physics. We are able to obtain reliable error bars for each estimate. The results are in excellent agreement with known exact calculation.

It has long been a hope in perturbative quantum field theory (PQFT), first expressed by Richard Feynman, to be able to estimate, in a given order, the result for the coefficient, without the brute force evaluation of all the Feynman diagrams contributing in this order. As one goes to higher and higher order, the number of diagrams, and the complexity of each, increases very rapidly. Feynman suggested that even a way of determining the sign of the contribution would be useful.

The standard model (SM) of particle physics seems to work extremely well. This includes quantum chromodynamics (QCD), the electroweak theory as manifested in the Weinberg–Glashow–Salam model, and quantum electrodynamics (QED). In each case, however, we must use perturbation theory and compute large numbers of Feynman diagrams. In most of these calculations, however, we have no idea of the size or sign of the result until the computation is completed.

Recently we proposed (Samuel *et al.*, 1993a,b, 1994; Samuel and Li, 1994a–c) a method to estimate coefficients in a given order of PQFT, without actually evaluating all of the Feynman diagrams in this order. In this paper, we present a method for obtaining reliable error bars for each estimate. We believe this makes our estimation method much more important and much more useful.

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Our method makes use of Padé approximants (PA) and gives us a Padé approximant prediction (PAP). There are many good references for PA; see, for example, Zinn-Justin (1971), Nutall (1970), Baker (1975), Bender and Orzag (1978), and Chlouber *et al.* (1992). We begin by defining the PA (type I)

$$(N, M) = \frac{a_0 + a_1 x + \cdots + a_N x^N}{1 + b_1 x + \cdots + b_M x^M} \tag{1}$$

to the series

$$S = S_0 + S_1 x + \cdots + S_{N+M} x^{N+M} \tag{2}$$

where we set

$$(N, M) = S + O(x^{N+M+1}) \tag{3}$$

We have written a computer program which solves equation (3) and then predicts the coefficient of the next term S_{N+M+1}. It works for arbitrary N and M. Furthermore, we have derived algebraic formulas for the $(N, 1)$, $(N, 2)$, $(N, 3)$, and $(N, 4)$ PAs, where N is arbitrary.

To illustrate the method, consider the simple example

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

We write the (1, 1) Padé as follows:

$$(1, 1) = \frac{a_0 + a_1 x}{1 + b_1 x} \tag{5}$$

It is easy to show that

$$a_0 = 1, \qquad b_1 = 2/3, \qquad a_1 = 1/6, \qquad c = 9/2$$

We can see that the prediction for c is close to the correct value $c = 4$. For $x = 1$, we get $(1, 1) = 7/10$, close to the correct result, $\ln 2 = 0.6931$. This is much better than the partial sum

$$1 - \frac{1}{2} + \frac{1}{3} = \frac{5}{6} = 0.8333 \tag{6}$$

If we now take the series

$$\frac{\ln(1 + x)}{x} = 1 - \frac{x}{2} + \frac{x^2}{3} - \frac{x^3}{4} \tag{7}$$

we have $S_0 = 1$, $S_1 = -1/2$, $S_2 = 1/3$, $S_3 = -1/4$, then

$$(1, 2) = \frac{a_0 + a_1 x}{1 + b_1 x + b_2 x^2}$$
$$= \frac{1 + x/2}{1 + x + x^2/6} \tag{8}$$

and for $x = 1$ we obtain

$$(1, 2) = 9/13 = 0.6923$$

very close to the correct value, ln 2 = 0.6931. (The partial sum is 0.58.) The PAP is

$$S_4(1, 2) = 7/36 = 0.1944 \tag{9}$$

very close to the correct value of 1/5.

The error bars are obtained by considering the magnitude of the coefficients $|S_n|$ (We use both S_n and $|S_n|$ and take the larger error.) First we consider the reciprocals

$$r_n = 1/s_n \tag{10}$$

find the PAP for r_{n+1}, and then take the reciprocal. This gives us an upper bound (UB). Then we consider the differences

$$t_n = r_{n+1} - r_n \tag{11}$$

and find the PAP for t_n. We then have

$$r_{n+1} = r_n + t_n \tag{12}$$

and then take the reciprocal

$$S_{n+1} = 1/r_{n+1} \tag{13}$$

This gives us a lower bound (LB). For the example above where $S_n = (n + 1)$ we find for the $r_n = 1/S_n$ method that the $(n - 1, 2)$ PAP for r_{n+2} has

$$\%\ \text{error} = \frac{-4}{(n + 1)^2(n + 2)^2} \tag{14}$$

and for the t_n method for r_{n+2}

$$\%\ \text{error} = \frac{+12}{n(n + 1)^2(n + 2)^2} \tag{15}$$

Thus the first method provides an UB for S_n and the second provides a LB. For the above example for $S_n = (n + 1)$ the UBs are

$$S_4 = 5.144 \quad \text{and} \quad S_5 = 6.0606 \tag{16}$$

Table I. PAP Estimates for the Difference $a_\mu - a_e$, the Anomalous Magnetic Moments of the Muon and Electron, respectively[a]

Estimate	$a_\mu - a_e$ error	Error 2/3 exact	|Estimate − exact|
705	275	570 ± 140	135
2499	482	—	—

[a] $a = (g - 2)/2$.

Table II. PAP Estimates for a_e

	a_e	Error 24	
−1.55	0.46	−1.434 ± 0.138	0.116
1.75	0.56	—	—

while the LBs are

$$S_4 = 4.69 \qquad \text{and} \qquad S_5 = 5.9418 \tag{17}$$

We take as our error here Δ, where Δ is the magnitude of the difference between equations (16) and (17). So our estimates for S_4 and S_5 are

$$S_4 = 5.00 \pm 0.45$$
$$S_5 = 6.00 \pm 0.12 \tag{18}$$

The estimates are exact in this case. We now generalize this procedure and take Δ as our error bars.

We now apply this method to several examples from QED, QCD, statistical physics, and mathematics. For odd $N + M$ we use the $(N, N + 1)$ and $(N + 1, N)$ PAPs, calculating an estimate and an error bar for each. For even $N + M$ we use (N, N), $(N - 1, N + 1)$, and $(N + 1, N - 1)$. We then combine the estimates for a given coefficient statistically.

In Table I we present the results for $a_\mu - a_e$, where $a = (g - 2)/2$ and a_e and a_μ are the anomalous magnetic moments of the muon and electron, respectively. Our result for tenth order is consistent with the known result and we give our prediction for 12th order:

$$a_\mu^{(12)} - a_e^{(12)} = 2499 \pm 482 \tag{19}$$

In Table II we present the estimates for a_e in eighth order and tenth order (Kinoshita, 1990). The result in eighth order

$$a_e^{(8)} = -1.55(46) \tag{20a}$$

is excellent and our estimate for tenth order is

$$a_e^{(10)} = 1.75 \pm 0.56 \tag{20b}$$

In Table III we present the results for the τ lepton (Samuel *et al.*, 1991), $a_\tau - a_e$. The results for tenth order and 12th order are excellent and our estimate for 14th order is

$$a_\tau^{(14)} - a_e^{(14)} = 27{,}427 \pm 3615 \tag{21}$$

The conservative approach would be to double all the error bars, using 2Δ instead of Δ for the error. However, these error bars are conservative and one can safely take $\Delta/2$ as the error bar in most cases. These errors should be considered as one standard deviation σ.

In Table IV we present the results for the five-loop β function in $g\phi^4$ theory (Kleinert *et al.*, 1991). The results for the four-loop and five-loop coefficients are very good and the estimate for the six-loop (unknown) coefficient is

$$\beta^{(6)} = -15{,}934 \pm 4588 \tag{22}$$

In Table V we present the results for the cumulative partitions of n into four nonzero integers, while Tables VII and VIII are for three and two integers,

Table III. PAP Estimates for $a_\tau - a_e$, where a_τ is the Anomalous Magnetic Moment of the τ Lepton

	$a_\tau - a_e$	Error 4/5	
1,997	795	1779	218
9,697	1601	8125	1572
27,427	3615	—	—

Table IV. PAP Estimates for the β-Function in $g\phi^4$ Theory

	$g\phi^4$ β-function	Error 10/11	
−94	42	−135.8	42
1,146	389	1424.3	278
−15,575	3660	—	—

Table V. PAP Estimates for Partitions into Four Integers

Estimate	Partitions (4) error	Error 18/19 exact	|Estimate − exact|
45.0	11.3	35	10
73.3	8.9	70	3.3
125.9	5.6	126	0.1
209.0	3.4	210	1.0
329.7	1.7	330	0.3
495.2	0.9	495	0.2
715.03	0.78	—	—

Table VI. PAP Estimates for the Spontaneous Magnetic Coefficients in the Honeycomb Lattice

Estimate	PAD 4 error	Error 41 exact	|Estimate − exact|
246.2	17	268	21.8
848.3	150	944	95.7
3,353	265	3,476	123
13,221	212	13,072	149
49,915	347	49,672	243
189,467	6406	—	—

Table VII. PAP Estimates for Partitions into Three Integers

	Parts (3)	Error 14/15	Parts
25	5.4	20	5
36.6	3.5	35	1.6
56.0	1.8	56	0
83.7	0.94	84	0.3
119.9	0.41	120	0.1
165.0135	0.185	165	0.0135
220.0037	0.072	220	0.0037
286	0.0306	286	0
364	0.0109	364	0
455	0.00445	—	—

Table VIII. PAP Estimates for Partitions into Two Integers

Estimate	Parts (2) Error	Error 16/17 Exact	|Estimate − exact|
15.6	1.1	15	0.6
21.1	0.43	21	0.1
27.95	0.183	28	0.05
35.989	0.067	36	0.01096
45	0.0258	45	0
55	0.0088	55	0
66	0.00329	—	—

respectively. The results can be seen to be very good. Tables VI and IX–XI are results from statistical physics (Domb and Green, 1974, 1979; Domb, 1974). All of these results are very good.

In Table XII we present the results for the number of partitions of n into nonzero positive integers. The results can be seen to be very good. Table XIII gives the PAP estimates for the R ratio in the $\overline{\text{MX}}$ scheme in perturbative quantum chromodynamics (PQCD). The four-loop estimate is $R(4) = -10.20 \pm 1.53$, in agreement with the known result, -12.805. Our estimate for the

Table IX. PAP Estimates for the Spontaneous Magnetic Coefficients in the Square Lattice

	PAD^3	Error 31	
679.5	105	714	34.5
3,449	325	3,472	23
17,256	612	17,318	60
87,903	123	88,048	150
454,080	350	454,380	300
2,373,100	1800	2,373,000	100
12,515,000	800	12,516,000	1000
66,549,000	2200	—	—

Table X. PAP Estimates for the Spontaneous Magnetic Coefficients in the Diamond Lattice

Estimate	PAD 1 error	Error 21 exact	|Estimate − exact|
522.7	40	534	11.3
1,709	39	1,732	23
5,710	36	5,706	4
19,028	54	19,038	10
64,157	101	64,176	19
218,200	63	218,190	10
747,052	51	747,180	128
2,574,496	100	—	—

Table XI. PAP Estimates for the PAD 5 Spontaneous Magnetization Coefficients for the Simple Cubic Lattice in the Ising Model

PAD 5 Estimate	Error	Exact	|Estimate − exact|
−2,127	657	−2,148	21
7,528	817	7,716	188
−22,882	181	−23,262	380
80,684	1078	—	—

five-loop result is $R(5) = -87.5 \pm 10.8$. The results for the MS scheme are given in Table XIV. Here the estimate for the four-loop result is extremely accurate and the error estimate is overly conservative. The five-loop estimate is 69.7 ± 48.9. Here, too, we expect that the error bound is overly pessimistic.

The corresponding results for the R_τ ratio in PQCD are given in Tables XV and XVI. The $\overline{\text{MX}}$ results in Table XV and the MS results in Table XVI for the four-loop coefficient are excellent, but here again our error bound is

Table XII. PAP Estimates for the Number of Partitions of n into Nonzero Positive Integers

Parts ($R_0 = 0$)			
4	2	3	1
4.4	0.8	5	0.6
8.5	1.6	7.0	1.5
12.3	2.1	11	1.3
15.4	1.3	15	0.4
40.2	5.4	—	—

Table XIII. PAP Estimates for the R Ratio in the $\overline{\text{MS}}$ Scheme in Perturbative QCD (PQCD) Number of Fermion Flavors (Quarks) $N_f = 5$

$R(t = 0)$ estimate	$\overline{\text{MS}}$ error	Exact	|Estimate − exact|
−10.20	1.53	−12.805	2.61
−87.5	10.8	—	—

Table XIV. PAP Estimates for the R Ratio in the MS Scheme in PQCD for $N_f = 5$

$R(t = 1.95)$	MS		
14.5	6.5	16.5	2.0
69.7	24.5	—	—

Table XV. PAP Estimates for the R_τ Ratio in the $\overline{\text{MS}}$ Scheme in PQCD for $N_f = 3$

$R_\tau(t = 0)$	$\overline{\text{MS}}$		
27.06	6.77	26.37	0.69
109.2	12.9	—	—

Table XVI. PAP Estimates for the R_τ Ratio in the MS Scheme in PQCD for $N_f = 3$

$R_\tau(t = 1.95)$	MS		
92.11	23.1	99.25	7.13
1026.8	251.0	—	—

very conservative. The estimates for the five-loop coefficients in the $\overline{\text{MS}}$ and MS schemes are $R_\tau^{(5)} = 109.2 \pm 12.9$ and 1026.8 ± 502.0, respectively.

In conclusion, we have presented a way of estimating perturbative coefficients with reliable error bars. We believe that this method will prove to be very useful in a wide variety of areas, especially in quantum electrodynamics (QED) and quantum chromodynamics (QCD), where calculations of the next-order terms are very difficult.

After this work was completed, we received a very interesting paper by Kataev and Starshenko (1994) in which they estimate the five-loop coefficients for R and R_τ by a completely independent method. These results in the $\overline{\text{MS}}$ scheme $R^{(5)} = -96.8$ and $R_\tau^{(5)} = 105.5$ are amazingly close to our results $R^{(5)} = -87.5 \pm 10.8$ and $R_\tau^{(5)} = 109.2 \pm 12.9$, respectively.

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