PSIpress
perfscipress.com
01 jan 10: A

Theory of box series

R.E. Crandall*

Abstract. By "box series" we speak of analytic series that at certain arguments yield the elusive box integrals $B_n(s)$, the latter being expectations $\langle |\vec{r}|^s \rangle$ where $\vec{r}$ ranges uniformly and randomly over the unit n-box. Remarkably, handling series coefficients according to a certain tableau allows fast computation of any $B_n(s)$, in fact to D good digits in only $O(n^2 D)$ operations, where the implied big-O constant depends only on s. As an example application of such a box-series algorithm, D. Bailey [1] has calculated a box integral of one million dimensions to > 100 decimal precision, which value starts out:

$$B_{1000000}(1) \;=\; 577.350211454572039977\ldots$$

We also give exact analytic forms for some box series, these in turn leading to closed-form box-integral evaluations.

*Center for Advanced Computation, Reed College, Portland OR, crandall@reed.edu.

R.E. Crandall, "Theory of box series,"
PSIpress, 01 jan 10: A, http://www.perfscipress.com/papers/FastBn_psipress.pdf

1 Box series defined

1.1 Motivation

The box series we define as

$$A_m(s,t) \;:=\; \sum_{k\geq 0} \gamma_{m,k}(s)\; t^k \tag{1}$$

where the γ coefficients are

$$\gamma_{m,k}(s) \;:=\; (-s/2)_k\, \beta_{m,k},$$

where $(a)_k = \Gamma(a+k)/\Gamma(a)$ is the Pochhammer symbol, while the β coefficients—defined below—arise from the theory of box integrals whose basic definition is

$$B_n(s) \;:=\; \int_{\vec{r}\in[0,1]^n} |\vec{r}|^s\; \mathcal{D}\vec{r}. \tag{2}$$

Thus B_n can be thought of as an expectation $\langle|\vec{r}|^s\rangle$ in the unit n-box.

A primary motive for the definition of the box series A is that for argument $t := 2/n$ we obtain a box integral of recent literature interest, as it has been shown that [2][3]:

$$B_n(s) = \frac{n^{1+s/2}}{s+n} A_{n-1}(s, 2/n). \tag{3}$$

So, in an obvious sense of generality, A_{n-1} is more profound than B_n.

It will turn out that careful inspection of the structure of the γ (or β) coefficients leads to a fast computational algorithm for the B_n. A side concern will be: When (for what t) does the series (1) converge? This question we shall answer with rigor, via bounds on the Pochhammer symbol.

1.2 Details on coefficients

The β numbers arising in the modern theory of box integrals can be defined in a number of ways, one of which being [2]

$$\beta_{mk} \;:=\; \frac{m^k}{2^k k!} \int_{\vec{r}\,\in\,[0,1]^m} \left(1 - \frac{r^2}{m}\right)^k \mathcal{D}\vec{r}. \tag{4}$$

These coefficients satisfy, for $m > 0, k \geq 1$ a recursion

$$(1 + 2k/m)\; \beta_{m,k} \;=\; \beta_{m,k-1} + \beta_{m-1,k} \tag{5}$$

ignited by $\beta_{0,k} := \delta_{0,k}$ and $\beta_{m,0} := 1$. This leads to an important recursion for the γ coefficients in the box series (1), again for $m > 0, k \geq 1$:

$$(1 + 2k/m)\; \gamma_{m,k} \;=\; (k - 1 - s/2)\, \gamma_{m,k-1} + \gamma_{m-1,k}. \tag{6}$$

With ignition $\gamma_{0,k} := \delta_{0,k},\ \gamma_{m,0} := 1$, the γ-recursion (6) serves three purposes:

1. Defines completely the box series (1),
2. Leads to a fast computational algorithm,
3. Implies some closed-form analytic evaluations.

2 Convergence properties

Being as convergence properties of a box series $A_m(s,t)$ depend on the growth of the coefficients $\gamma_{m,k}(s)$, we begin with a universal, effective bound:

Lemma 1 [Effective bound on Pochhammer symbol] *For any complex a there exists a real number $C(a)$ such that for all positive integers k we have a bound*

$$|(a)_k| \;\le\; C(a)\,(k-1)!\;k^{\Re(a)}.$$

Moreover, for given a, the factor $C(a)$ can be effectively computed.

Proof: Define

$$C_k(a) \;=\; \frac{|(a)_k|}{(k-1)!\;k^{\Re(a)}}.$$

We wish to show that $C_k(a)$ is bounded as $k \to \infty$. First, for positive integers k_0, M,

$$C_{k_0+M}(a) \;=\; C_{k_0}(a) \prod_{k=k_0}^{k_0+M-1} \left|1+\frac{a}{k}\right| \left(\frac{k}{k+1}\right)^{\Re(a)}.$$

Now we can bound any of the multiplicands by assigning $k_0 := \lceil 2|a|+3 \rceil$ and assuming $k \ge k_0$:

$$\begin{aligned}\left|1+\frac{a}{k}\right| \left(\frac{k}{k+1}\right)^{\Re(a)} \;&=\; e^{\Re(\log(1+a/k))}e^{-\Re(a)\log(1+1/k)} \\ &\le e^{\frac{1}{2}\frac{|a|^2}{k^2}\frac{1}{1-|a|/k}}\,e^{\frac{1}{2}\frac{|a|}{k^2}\frac{1}{1-1/k}} \\ &\le e^{\frac{|a|^2+|a|}{k^2}}.\end{aligned}$$

It follows that

$$C_{k_0+M} \;\le\; C_{k_0}e^{|a|/2},$$

so not only is $C_k(a)$ bounded, but we have an effective bounding factor (recall k_0 depends on a only)

$$C(a) \;:=\; C_{k_0}(a)e^{|a|/2}.$$

QED

Lemma 1 establishes—rather simply, from the bound within said lemma and the representation (4)—the result:

Theorem 1 **[Convergence theorem for box series]** *For any complex s and integers $m, k \geq 0$ we have a coefficient bound*

$$|\gamma_{m,k}| \;\leq\; C\left(-\frac{s}{2}\right)\left(\frac{m}{2}\right)^k k^{-1+\Re(s)/2}.$$

Accordingly, the box series $A_m(s,t)$ defined by (1) is absolutely convergent whenever

$$|t| < \frac{2}{m}.$$

In turn, we now know how quickly the series (3) converges to the relevant box integral:

Corollary 1 **[Box-integral convergence]** *The series (3), written here as*

$$B_n(s) \;=\; \frac{n^{1+s/2}}{s+n}\sum_{k\geq 0}\gamma_{n-1,k}(s)\left(\frac{2}{n}\right)^k$$

is absolutely convergent for all complex s and positive integer $n \neq -s$. Moreover, the k-th summand is bounded by

$$C\left(-\frac{s}{2}\right)\left(1-\frac{1}{n}\right)^k.$$

3 Fast computational algorithm for B_n

From Corollary 1 we infer that D good digits of a box integral $B_n(s)$ can be obtained via $O(nD)$ summands, with the implied big-O constant depending only on s. It turns out that we can evaluate a coefficient $\gamma_{m,k}(s)$—for any k—in an average of $O(n)$ operations per coefficient; thus, the claim in our Abstract holds, namely

$$O(n^2 D)$$

operations suffice to resolve $B_n(s)$ to D digits.

The relevant algorithm runs like so:

Algorithm 1 [Fast computation of box series and box integrals] This algorithm calculates box series $A_{n-1}(s,t)$ or box integral $B_n(s)$.

1. Define $m := n-1$ and initialize a coefficient vector $(\gamma_{1,0}, \gamma_{2,0}, \ldots, \gamma_{m,0}) := (1, 1, 1, \ldots, 1)$. Also set $A := p := 1$. If box series is desired we assume t given; else, if box integral is desired, set $t := 2/n$.

2. for($k = 1$; ; k++) {

    $\sigma := (k - 1 - s/2)$;

    // Next, update the coefficient vector (to be done in-place; no vector copies needed):

    $\gamma_{1,k} := \frac{\sigma}{1+2k}\gamma_{1,k-1}$;

    for($\mu = 2$; $\mu \le m$; μ++) $\gamma_{\mu,k} = \frac{\sigma\,\gamma_{\mu,k-1} + \gamma_{\mu-1,k}}{1+2k/\mu}$;

    $p * = t$;

    $A + = \gamma_{m,k} * p$;

    }

3. Return $A_m(s,t)$ as A, or box integral $B_n(s)$ as $A \cdot n^{1+s/2}/(s+n)$.

It would be an interesting research matter to compare this fast algorithm against the mighty quadrature apparatus used by D. Bailey and A. Kaiser in recent computations on the B_n integrals [3]. In any case it must be remembered that said quadrature methods opened up the door to new box-integral discoveries, even theoretical ones, and in that sense are historically irreplaceable.

An interesting feature of Algorithm 1 is that it can give *rigorous* upper or lower bounds, simply because the Pochhammer symbol $(-s/2)_k$ for real s is eventually positive, and so $\gamma_{m,k}(s)$ is eventually positive for sufficiently large k. In this way, one could in principle test quadrature schemes via bounding observations for the box series A.

Though extensive tests have not been carried out for Algorithm 1, one may calculate $B_{1000000}(1)$ as in our Abstract. This was done using 120-digit precision via Algorithm 1. D. Bailey's actual value is

$$B_{1000000}(1) \approx 577.35021145457203997753408752036227457448125926146101942964$$
$$79537136802898037940751957186734998792562783929529634543349639,$$

presumably correct to at least 100 decimal places. We have not worked out any rigorous accuracy estimates for this box integral; however, it is satisfying to see how efficient is Algorithm 1 in practice.

Incidentally, the numerical efficiency of Algorithm 1 can be better than expected, for the following reason. As we have argued, using $m := n-1$ summands of (1), each requiring $O(m)$ operations in Algorithm 1's main loop, yields the $O(n^2 D)$ estimate for D good digits. However, the proof of Theorem 1 used the integral (4), in the sense that

$$\beta_{m,k} \le \frac{m^k}{2^k k!},$$

and yet, a tighter estimate is achieved by noting $(1 - r^2/m)^k \le e^{-kr^2/m}$, so that actually

$$\beta_{m,k} \le \frac{m^k}{2^k k!} \left(\frac{\sqrt{\pi}\,\mathrm{erf}\left(\sqrt{k/m}\right)}{2\sqrt{k/m}} \right)^m .$$

Thus, one could, if one wished, insert the erf-power factor here into the bound for $|\gamma_{m,k}|$ in Theorem 1. Such a factor does not change the asymptotics for really large digit count D, but for the initial digits of accuracy, the convergence is satisfying. More quantitatively, though we have obtained $B_{1000000}(1)$ to accuracy $D \approx 10$, we did not need anywhere near $n^2 D \approx 10^{13}$ operations. (Alternatively, we did not need $k \approx 10^6$ terms; we used 10^3 terms.) However, if $D >> n$, the estimate $O(n^2 D)$ is more realistic in practical terms..

4 Closed analytic forms

It follows from the recursion (6) that the box series satisfies the differential equation

$$\left(1 + \frac{s}{2} t\right) A_m(s,t) + \left(\frac{2}{m} t - t^2\right) \frac{\partial}{\partial t} A_m(s,t) \;=\; A_{m-1}(s,t). \tag{7}$$

Remarkably, this leads to a formal integral recursion

$$A_m(s,t) \;=\; \frac{\left(\frac{2}{m} t - t\right)^{(s+m)/2}}{t^{m/2}} \int_0^t A_{m-1}(s,\tau) \frac{\tau^{m/2-1}}{\left(\frac{2}{m} - \tau\right)^{1+(s+m)/2}} \, d\tau. \tag{8}$$

This integral relation is far more than a curiosity, for various exact analytic resolutions arise immediately.

We know from the very definition of the γ coefficients that

$$A_0(s,t) \;=\; 1.$$

Using this in the integral recursion (8) we then have

$$A_1(s,t) \;=\; {}_2F_1\left(1, -\frac{s}{2}; \frac{3}{2}; \frac{t}{2}\right).$$

Incidentally, since $\beta_{1,k} = 1/(2k+1)!!$, this A_1 resolution also follows from symbolic evaluation of $\sum_{k\geq 0}(-s/2)_k t^k/(2k+1)!!$ as the indicated hypergeometric. In any case, this A_1 form leads to the known hypergeometric form for B_2 [3]:

$$B_2(s) \;=\; \frac{2}{2+s}\,{}_2F_1\left(\frac{1}{2},-\frac{s}{2};\frac{3}{2};-1\right).$$

True difficulties start to appear for $m = 2$. We do not know a general closed hypergeometric form for $A_2(s,t)$.[1] However, there are cases that follow from the integral recursion (8), e.g.

$$t\,A_2(-2,t) \;=\; -2\mathrm{G} - i\mathrm{Li}_2\left(-it - \sqrt{-(t-2)t} + i\right) + i\mathrm{Li}_2\left(i(t-1) + \sqrt{-(t-2)t}\right) - 4i\sin^{-1}\left(\frac{\sqrt{t}}{\sqrt{2}}\right)\tan^{-1}\left(-t + i\sqrt{-(t-2)t} + 1\right).$$

Here, G is the Catalan constant, and of course the whole expression must be real for real t, so in such cases real parts can be taken for any term(s). This evaluation leads eventually—for argument $t := 2/3$—to the known resolution

$$B_3(-2) \;=\; -3\mathrm{G} + \frac{3}{2}\pi\log(1+\sqrt{2}) + 3\;\;\mathrm{Ti}_2(3-2\sqrt{2}),$$

where Ti is the Lewin-arctan integral [3].[2]

We do not know any closed forms for $A_3(s,t)$ *except* in the case $t = 1/2$. That is, we can put any $A_3(\text{integer}, 1/2)$ into closed form, by virtue of all $B_4(\text{integer})$ being hyperclosed (see [3] for definition of hyperclosure as well as sample B_4 closures.) Similarly, some—but all—of the cases $A_4(\text{integer}, 2/5)$ are hyperclosed, by virtue of knowledge of a great many $B_5(\text{integer})$ [3].

In spite of the obstacles standing in the way of high-dimension evaluations of box series, we do know *some* exact evaluation of A_m in *any* dimension m. For example, it is evident (see the B_n expansion in Corollary 1) that $B_n(s)$ has a single pole in the complex s-plane, and that this pole is at $s = -n$. From knowledge of the residues at such poles—which knowledge is subsequent to the research in [3]—we deduce a rather peculiar yet exact box-series evaluation

$$A_{n-1}\left(-n, \frac{2}{n}\right) = \frac{n^{n/2-1}}{2^{n-1}}\frac{\pi^{n/2}}{\Gamma(n/2)}.$$

Just one check of this arbitrary-dimension evaluation uses the instance

$$A_1(-2,t) \;=\; \frac{2\sin^{-1}\left(\sqrt{t/2}\right)}{\sqrt{(2-t)t}},$$

[1] It does appear, though, that one can obtain a closed $A_2(s,t)$ for any integer $s \leq 0$.

[2] How to go from the Li form for $A_2(-2,2/3)$ to the known $B_3(-2)$ form was found and communicated by J. Borwein. (Lewin polylogarithm and arctan-integral identities are involved.)

whence

$$A_1(-2,1) \;=\; \frac{\pi}{2}$$

as expected. Another example runs:

$$A_2(-3,t) \;=\; \frac{\pi - 4\tan^{-1}\left(\sqrt{1-t}\right)}{t\sqrt{1-t}},$$

whence

$$A_2(-3,2/3) \;=\; \pi\frac{\sqrt{3}}{2}.$$

5 Acknowledgments

The author is grateful to D. Bailey and J. Borwein for collegial research—past and present—on box integrals.

References

[1] D. Bailey, private communication (2009).

[2] D. Bailey, J. Borwein, and R. Crandall, "Box integrals," *Journal of Computational and Applied Mathematics* 206 (2007) 196-208.

[3] D. Bailey, J. Borwein, and R. Crandall, "Advances in the theory of box integrals," preprint, 2009.