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NOTE

Accurate Normalisation of the Beta-Function PDF

The beta-function probability density function (pdf) [1] is often chosen to model turbulent scalar mixing, both in inert and reactive flows. The pdf is defined by

$$p(x) = \frac{x^{\beta_1 - 1}(1 - x)^{\beta_2 - 1}}{B_\infty}, \tag{1}$$

where the beta function B_∞ is defined by

$$B_\infty = \int_0^1 x^{\beta_1 - 1}(1 - x)^{\beta_2 - 1}\, dx. \tag{2}$$

The two parameters β_1 and β_2 must be positive and are related to the mean μ and root mean square σ of $p(x)$ by

$$\beta_1 = \mu \left[\frac{\mu(1 - \mu)}{\sigma^2} - 1\right], \tag{3}$$

$$\beta_2 = (1 - \mu) \left[\frac{\mu(1 - \mu)}{\sigma^2} - 1\right]. \tag{4}$$

The beta function may also be computed using the standard Gamma function by means of

$$B_\infty = \frac{\Gamma(\beta_1)\Gamma(\beta_2)}{\Gamma(B_1 + \beta_2)}, \tag{5}$$

where

$$\Gamma(z) = (z - 1)! = \int_0^\infty t^{z-1} e^{-t}\, dt. \tag{6}$$

It is difficult to compute B_∞ using numerical techniques when β_1 and/or β_2 are below unity, because the integrand of Eq. (2) is ill conditioned for numerical integration; both the integrand and its slope are infinite at one or both ends, as shown in the example of Fig. 1. For this type of function the usual techniques (mid-point rule, Simpson's rule, Gaussian quadrature) yield unsatisfactory results [2]. Moreover, the integrand may itself overflow or underflow floating-point operations, even when using double-precision arithmetic.

Using polynomial expansions of $\Gamma(z)$, such as those given in [3], with Eq. (5) will not yield much improvement since the polynomials are not accurate at very low values of z; under and overflow problems are also present.

Takahashi and Mori [4] have studied the related function,

$$\int_{-1}^1 (1 + z)^{\beta_1 - 1}(1 - z)^{\beta_2 - 1} f(z)\, dz. \tag{7}$$

(This may be transformed into Eq. (2) by the substitution $1 + z = 2x$ and making $f(x) = 2^{1-\beta_1-\beta_2}$.)

To compute this function Takahashi and Mori [4] used the substitution

$$z = \frac{2}{\sqrt{\pi}} \int_0^u e^{-t^2}\, dt = \operatorname{erf} u, \tag{8}$$

which transforms (7) into

$$\frac{2}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2} (1 + \operatorname{erf} u)^{\beta_1 - 1} (1 - \operatorname{erf} u)^{\beta_2 - 1} f(\operatorname{erf} u)\, du. \tag{9}$$

This integrand is better conditioned, exhibiting zero slope at $u = \pm\infty$, but this is achieved at the expense of an infinite integration domain, which necessitates a large number of points.

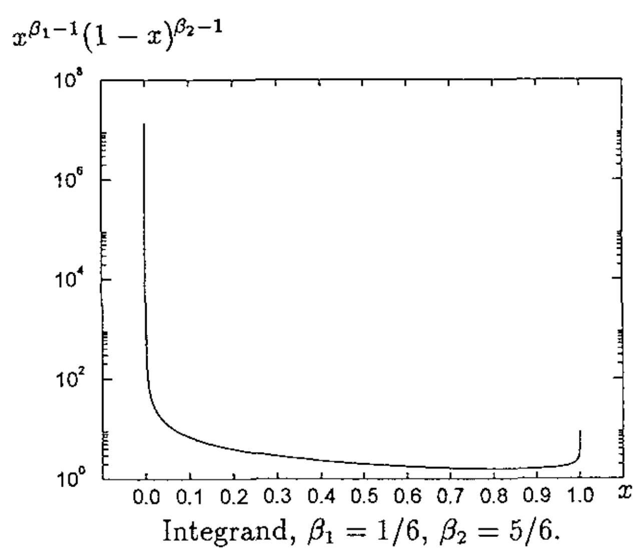

FIGURE 1

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TABLE I

Beta Functions

β_1	β_2	μ	σ	Eq. (12)	Exact B_∞	Error
10^{-4}	10^{-4}	0.5000	0.4999	20001	20000[a]	50 ppm
10^{-4}	10^{-2}	0.0099	0.0985	10100.48	10100.01[a]	46 ppm
$\frac{1}{6}$	$\frac{5}{6}$	0.1666	0.2635	6.283309	2π[b]	19 ppm
1	1	0.5000	0.3535	1.000000	1	0 ppm
11	21	0.3437	0.0827	1.073658×10^{-9}	1.073658×10^{-9}[c]	0 ppm

[a] Approximate formula, Eq. (16).
[b] Using reflection formula $\Gamma(x)\Gamma(1-x) = \pi/\sin \pi x$, whence $B_\infty = \Gamma(\frac{1}{6})\Gamma(\frac{5}{6})/\Gamma(\frac{1}{6}+\frac{5}{6}) = \pi/\sin \pi/6$.
[c] Using $B_\infty = \Gamma(11)\Gamma(21)/\Gamma(32) = 1/(5 \times 7 \times 9 \times 11 \times 13 \times 23 \times 29 \times 31)$.

It is desired to find a technique to compute the Beta function for low values of the parameters which is better conditioned for numerical integration, utilizes a finite integration interval, and is accurate. Using the recurrence formula

$$\Gamma(1+x) = x\Gamma(x), \tag{10}$$

we can put

$$\Gamma(\beta) = \frac{\Gamma(\beta+1)}{\beta} = \frac{\Gamma(\beta+2)}{\beta(1+\beta)}. \tag{11}$$

Hence, using Eqs. (2) and (5) it is not difficult to show that

$$B_\infty = \frac{(\beta_1+\beta_2)(\beta_1+\beta_2+1)(\beta_1+\beta_2+2)(\beta_1+\beta_2+3)}{\beta_1\beta_2(1+\beta_1)(1+\beta_2)} \frac{\Gamma(\beta_1+2)\Gamma(\beta_2+2)}{\Gamma(\beta_1+\beta_2+4)}$$

$$= \frac{(\beta_1+\beta_2)(\beta_1+\beta_2+1)(\beta_1+\beta_2+2)(\beta_1+\beta_2+3)}{\beta_1\beta_2(1+\beta_1)(1+\beta_2)} \int_0^1 x^{\beta_1+1}(1-x)^{\beta_2+1}\,dx. \tag{12}$$

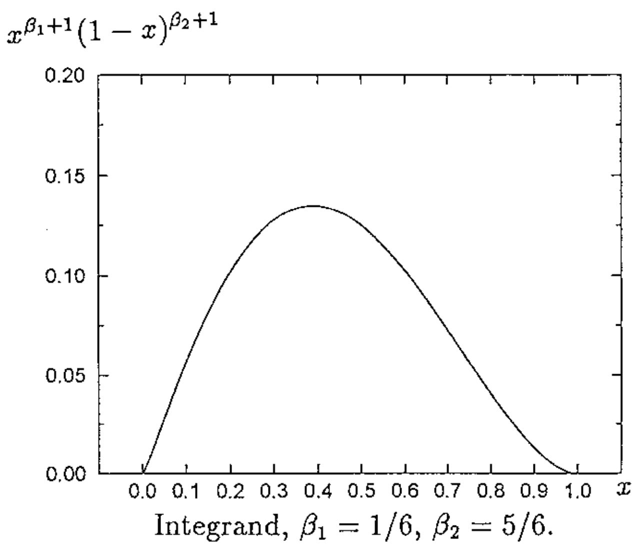

FIGURE 2

The last integral is much better suited to numerical integration since the integrand is zero at both ends with zero slope, as shown in the example of Fig. 2. For $0 < \beta_1 < 1$ and $0 < \beta_2 < 1$ the integrand has one simple maximum between $x = \frac{1}{3}$ and $x = \frac{2}{3}$, and this maximum ranges between $\frac{1}{16}$ and $\frac{1}{4}$. Equation (12) is not restricted to parameter ranges below unity.

When β_1 and β_2 are very small the integral tends to $\frac{1}{6}$, and we can approximate

$$B_\infty \simeq \frac{\beta_1+\beta_2}{\beta_1\beta_2}. \tag{13}$$

For comparison, at $z = 1$ the slope of the gamma function is approximately -1 (see, for instance, [3]), and for small x we can expand in a Taylor series:

$$\Gamma(z) = \Gamma(1+x) \simeq \Gamma(1) + x\frac{d\Gamma}{dz}\bigg]_{z=1} \simeq 1 - x. \tag{14}$$

Hence, using the recurrence formula we can approximate

$$\Gamma(x) = \frac{1-x}{x}. \tag{15}$$

Substituting Eq. (15) into Eq. (5),

$$B_\infty = \frac{\beta_1+\beta_2}{\beta_1\beta_2}\left(1 + \frac{\beta_1\beta_2}{1-\beta_1-\beta_2}\right) \simeq \frac{\beta_1+\beta_2}{\beta_1\beta_2}, \tag{16}$$

which agrees with Eq. (13).

Table I shows examples that are computed using Eq. (12) and the simplest algorithm, midpoint integration using 100 equal intervals. The results show the new formula is extremely accurate.

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