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Fitting human exposure data with the Johnson S_B distribution

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Exposure evaluations for epidemiological investigations and risk assessments may require estimates of background concentrations and peak exposures, as well as the population mean and variance. The S_B distribution is a theoretically appealing probability function for characterizing ratios, and random variables bound by extremes, such as human exposures and environmental concentrations. However, fitting the parameters of this distribution with maximum likelihood methods is often problematic, and some alternative methods are examined here. Two methods based on percentiles, a quantile estimator, and a method-of-moments fitting procedure are explored. The quantile and method-of-moments procedures are based on new explicit expressions for the first four moments of this distribution. The fitting procedures are compared by simulation, and with actual data sets consisting of measurements of human exposure to airborne contaminants.
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Introduction

The risk of disease from exposure to hazardous airborne contaminants is generally thought to be a function of the inhaled dose. This is inferred from quantitative exposure assessments and the application of exposure models. Epidemiological inquiries and risk assessments require a statistical characterization of the population exposure, and this leads to exploring the suitability of various probability distributions. Exposures are expressed as average concentrations and as such are bound by maximum and minimum values, and can always be expressed as a ratio. Some recent papers have explored the beta distribution (Flynn, 2004a, b) and the S_B distribution (Flynn, 2004c) as models for human exposure data, based on these constraints.

The Johnson S_B distribution, or alternatively the 4-parameter lognormal model, is appealing on theoretical grounds as a candidate probability distribution function for ratios, or variates constrained by extremes. It has found application in a variety of fields including ambient air pollution (Mage, 1980), rainfall distribution (Kottegoda, 1987) and forestry (Zhang et al., 2003). The distribution has also been applied to occupational exposures, and confidence intervals for the mean were estimated with a parametric bootstrap technique (Flynn, 2004c). This distribution was described in a classic paper (Johnson, 1949) that considered a variety of transformations on random variables that ultimately led to normal distributions. A more recent summary can be found in (Johnson et al., 1994). The S_B distribution, although flexible and appealing on first principles, is complex mathematically and estimation has been somewhat problematic.

The Johnson S_B distribution transforms a bounded random variable by subtracting the minimum and dividing by the range. The logit of this transformation is then distributed as a standard normal variable. Following Johnson (1949), consider this transform y on the random variable x:

$$y = \frac{x - \xi}{\lambda} \tag{1}$$

where ξ is the minimum value of x, $\xi + \lambda$ is the maximum value of x.

Within our context x is an exposure measurement, that is, a time-weighted average or instantaneous concentration. A unit normal variable z is defined as

$$z = \gamma + \delta \ln\left(\frac{y}{1-y}\right) = \gamma + \delta \ln\left(\frac{x-\xi}{\xi + \lambda - x}\right) \tag{2}$$

When minimum and maximum values are known *a priori*, maximum likelihood estimates for gamma and delta are

$$\hat{\gamma} = -\frac{\bar{f}}{s_f} \quad \text{and} \quad \hat{\delta} = \frac{1}{s_f} \quad \text{where}$$
$$f = \ln\left(\frac{y}{1-y}\right)$$

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and $\bar{f}$ is the sample mean and

$$s_f = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(f_i - \bar{f})^2} \quad (3)$$

When the extremes are not known *a priori*, the estimation process becomes more difficult, particularly when all four parameters are to be estimated. In this case maximum likelihood methods have not been particularly useful (Lambert, 1970; Vroon, 1981). Tsionas (2001) states — "the likelihood may have extremely fat tails, which is responsible for the absurd values that parameters often assume in maximum likelihood estimation".

Estimation based on sample percentiles appears particularly convenient, and two explicit methods have been reported, one by Slifker and Shapiro (1980), and the other by Mage (1980). Johnson and Kitchen (1971) describe a method-of-moments fitting procedure based on calculating the sample coefficients of skewness and kurtosis and using a look-up table for estimating gamma and delta. The range and minimum are then estimated directly by

$$\lambda = \frac{\sigma_x}{\sigma_y} \quad (4)$$

$$\varepsilon = \mu_x - \lambda\mu_y \quad (5)$$

This procedure formed the basis of an algorithm presented by Hill et al. (1976), which used a Newton–Raphson iterative scheme to estimate gamma and delta. This algorithm calculates the first six moments of the distribution by an approximate numerical integration technique. An example illustrating the use of the code to fit the S_B distribution was not given. Wheeler (1980) presented quantile estimators for gamma and delta, similar to the percentile methods but including the sample median in the estimation process. A specific procedure for estimating the extremes was not included.

Siekierski (1992) conducted a computer simulation study to compare three different methods for fitting S_B distributions to forestry data. A conditional maximum likelihood (CML) method, a modified method-of-moments, and a modified percentile method were explored. The modifications amounted to guessing the extreme values based on some *ad hoc* procedures. In the percentile approach the sample minimum was set to the zero percentile value. In the modified method-of-moments, the population minimum was estimated by the sample minimum minus one, and the population range was estimated as the sample range plus two. The study involved several thousand simulations from three different populations with sample sizes of 20, 100 and 500. Siekierski (1992) concludes that the maximum likelihood method does not always produce reasonable results, and recommends the modified method-of-moments approach. A more recent examination (Zhang et al. 2003) of fitting forestry data with the S_B distribution also employed *ad hoc* procedures similar to those of Siekierski (1992) for estimating the minimum values.

This work presents a variation on an existing algorithm (Hill et al., 1976) for estimating all four parameters of the S_B distribution based upon the method-of-moments outlined by Johnson and Kitchen (1971). Instead of a table look-up process, a computer program has been written to estimate gamma and delta given sample values of the coefficients of skewness and kurtosis. The program uses a Newton iteration subroutine (the IMSL subroutine DNEQNF), which calculates a finite difference approximation for the Jacobian. Unlike (Hill et al., 1976) this requires only the first four moments, which are calculated according to the analytic series formulas presented in Flynn (2005). This method of estimation is compared with the percentile methods of Slifker and Shapiro (1980), Mage (1980), and the quantile method of Wheeler (1980). The quantile method produces estimates of gamma and delta, epsilon and lambda are then estimated using equations (4) and (5) with the first two moments calculated by explicit formulas given in the Appendix A. Some illustrations are given with actual exposure data sets.

Methodology

In what follows subscripts on the unit normal (z), and the corresponding sample value (x) are from low to high values with the exception that the median has a zero subscript. The percentile methods of fitting have been described in detail by Mage (1980), and Slifker and Shapiro (1980). The latter method requires symmetric percentiles, while the former is a bit more flexible. For both methods used here the sample percentiles selected were symmetric at $\pm z$ and $\pm 3z$ with $z = 0.5384$ corresponding, approximately to the 30th, 70th, 5th and 95th percentiles.

For Mage's method (1980) the parameter estimates are:

$$\begin{aligned}
\hat{\varepsilon} &= -\frac{\phi}{2} - \sqrt{\frac{\phi^2}{4} - \theta} \\
\hat{\lambda} &= 2 - \sqrt{\frac{\phi^2}{4} - \theta} \\
\hat{\gamma} &= z_1 - \hat{\delta}\log\left(\frac{x_1 - \hat{\varepsilon}}{\hat{\lambda} + \hat{\varepsilon} - x_1}\right) \\
\hat{\delta} &= \frac{(z_2 - z_1)}{\log\left((x_2 - \hat{\varepsilon})(\hat{\lambda} + \hat{\varepsilon} - x_1)/(\hat{\lambda} + \hat{\varepsilon} - x_2)(x_1 - \hat{\varepsilon})\right)}
\end{aligned} \quad (6)$$

where

$$\begin{aligned}
\phi &= \frac{cd - ae}{bd - ae} \\
\theta &= \frac{ce - bf}{bd - ae} \\
a &= x_2 - x_4 - 2x_3 \\
b &= x_3^2 - x_2x_4 \\
c &= 2x_2x_3x_4 - (x_2 + x_4)x_3^2
\end{aligned}$$

$$\begin{aligned} d &= x_1 + x_3 - 2x_2 \\ e &= x_2^2 - x_1x_3 \\ f &= 2x_1x_2x_3 - (x_1 + x_3)x_2^2 \end{aligned} \tag{7}$$

For Slifker and Shapiro's method (1980), the parameter estimates are

$$\begin{aligned} \hat{\varepsilon} &= \frac{x_3 + x_2}{2} - \frac{\hat{\lambda}}{2} + \frac{p((p/n) - (p/m))}{2((p^2/mn) - 1)} \\ \hat{\lambda} &= \frac{p\sqrt{\{(1 + p/m)(1 + p/n) - 2\}^2 - 4}}{(p^2/mn) - 1} \\ \hat{\gamma} &= \hat{\delta}\ \sinh^{-1}\left[\frac{(p/n - p/m)\sqrt{(1 + p/m)(1 + p/n) - 4}}{2(p^2/mn - 1)}\right] \\ \hat{\delta} &= \frac{z}{\cosh^{-1}(1/2\sqrt{(1 + p/m)(1 + p/n)})} \end{aligned} \tag{8}$$

where

$$\begin{aligned} m &= x_4 - x_3 \\ n &= x_2 - x_1 \\ p &= x_3 - x_2 \end{aligned} \tag{9}$$

The quantile estimation procedure described by Wheeler (1980) provides estimates for gamma and delta. The sample median is used along with four additional percentile values at $\pm z$ and $\pm z/2$, where z is determined as a function of the sample size N by

$$F(z_n) = (n - 0.5)/N \quad \text{for}\, n \leq N$$

and F is the standard normal distribution function.

Parameter estimates are obtained here as

$$\begin{aligned} \hat{\gamma} &= -\hat{\delta}\log(A) \\ \hat{\delta} &= \frac{z_N}{2\log(B)} \end{aligned} \tag{10}$$

where

$$\begin{aligned} A &= \frac{t - B^2}{1 - tB^2} \\ B &= \frac{t_b}{2} + \sqrt{\left(\frac{t_b}{2}\right)^2 - 1} \\ t &= \frac{x_4 - x_0}{x_0 - x_1} \\ t_b &= \frac{(x_3 - x_0)(x_4 - x_1)}{(x_4 - x_3)(x_0 - x_1)} \end{aligned} \tag{11}$$

To examine the fitting methods described above two separate studies were conducted. The first involved taking 20 random samples: 10 of size $N = 50$ and 10 of size $N = 25$ from an S_B population with parameters representative of occupational exposure data. For each parameter estimate the mean and standard deviation of the 10 samples were calculated. In addition, a Shapiro–Wilk goodness-of-fit test statistic (W), and its associated P-value, were calculated for each sample. In the second study actual human exposure data from the literature were fit to the S_B distribution. In addition to the methods listed above, a CML method was also explored in this second study by setting the minimum exposure to 0 *a priori* and using the percentile approach originally suggested by Johnson (1949) to estimate the maximum. This approach has been used previously (Flynn, 2004c) for exposure data when the *a priori* minimum is set to 0. The data sets used here consist of personal breathing-zone exposure monitoring results and were: A — 33 samples for benzene taken from petrochemical workers (Tolentino et al., 2003); B — 55 total-mass spray-painting exposures (Carlton and Flynn, 1997); C — 27 isopropyl alcohol exposures in an automobile assembly plant (George et al., 1995); and D — 13 carbon dioxide exposures in the poultry industry (Jacobs and Smith, 1988).

Results

Tables 1 and 2 summarize the results from the simulation comparisons. The percentile methods give comparable performance. Each failed to obtain parameter estimates for two of the samples at $N = 50$: and for three of the samples at the $N = 25$ sample size. These methods each had multiple additional failures with the Shapiro–Wilk fit tests. They underestimate gamma and lambda, and overestimate delta and epsilon. The quantile method and the method-of-moments are also comparable. They each failed to obtain parameter estimates on only one sample regardless of sample size, and had no additional failures in the fit tests. They give more accurate and precise parameter estimates than do the percentile methods, and better fit the data, as the Shapiro–Wilk (W) statistics indicate. Based on these limited results, and the general agreement with the more detailed study by Siekierski (1992), the percentile methods were not considered further here.

Results from fitting actual data sets are shown in Table 3. At least one fitting method was successful, and for data set B all three procedures produced parameter estimates. Both the method-of-moments and the quantile fitting procedures failed for data set A. The CML method with *a priori* minimum set to zero failed in two cases. In all cases where a fit was obtained, the Shapiro–Wilk tests indicate that the null hypothesis of the sample being drawn from an S_B distribution could not be rejected.

Table 4 presents the comparison between the various fitting results and the sample values for the mean, standard deviation, minimum, and range. The method-of-moments and the quantile approach fit epsilon and lambda so that the sample mean and variance are matched exactly. A minor

Table 1. Mean and (standard deviation) for parameter estimates based on 10 random samples of size 50 from the test population.

	Gamma	Delta	Lambda	Epsilon	*W*
Slifker and Shapiro	0.54 (0.37)	1.80 (1.73)	7.14 (4.84)	0.40 (0.47)	0.39 (0.50)
Mage	0.52 (0.39)	1.96 (1.85)	6.72 (3.88)	0.33 (0.25)	0.49 (0.52)
Quantile	1.18 (0.71)	1.07 (0.37)	11.5 (3.94)	0.16 (0.21)	0.98 (0.004)
Method of moments	0.82 (0.50)	0.94 (0.28)	9.67 (2.68)	0.17 (0.19)	0.98 (0.01)
Population parameters	1.0	1.0	10.0	0.1	—

Table 2. Mean and (standard deviation) for parameter estimates based on 10 random samples of size 25 from the test population.

	Gamma	Delta	Lambda	Epsilon	*W*
Slifker and Shapiro	0.62 (0.50)	2.13 (2.75)	9.38 (12.3)	0.61 (0.66)	0.31 (0.47)
Mage	0.54 (0.44)	2.75 (1.85)	7.21 (5.75)	0.44 (0.48)	0.75 (0.42)
Quantile	1.40 (2.32)	1.07 (0.87)	15.0 (19.7)	0.33 (0.30)	0.96 (0.02)
Method of moments	0.72 (0.51)	0.89 (0.31)	9.20 (2.92)	0.31 (0.37)	0.96 (0.02)
Population parameters	1.0	1.0	10.0	0.1	—

Table 3. Parameter estimates and goodness-of-fit for the exposure data sets A–D.

Data ID	Parameter estimates and Shapiro–Wilk test	Quantile method	Method of moments	Conditional maximum likelihood (minimum = 0)
A	Gamma	No fit	No fit	1.61
Benzene	Delta			0.6983
	Lambda (ppm)			1.86
	Epsilon (ppm)			0 — set *a priori*
	W			0.98
	P			0.87
B	Gamma	1.81	1.51	1.38
Spray paint	Delta	0.86	0.75	0.7684
	Lambda (mg/m^3)	895.0	745.6	681.2
	Epsilon (mg/m^3)	0.0	4.06	0 — set *a priori*
	W	0.98	0.98	0.99
	P	0.87	0.91	0.92
C	Gamma	0.63	1.07	No fit
Isopropyl alcohol	Delta	0.79	0.93	
	Lambda (ppm)	51.4	63.06	
	Epsilon (ppm)	36.1	36.47	
	W	0.95	0.94	
	P	0.33	0.15	
D	Gamma	4.34	1.55	No fit
Carbon dioxide	Delta	1.83	1.09	
	Lambda (ppm)	102421.6	33138.3	
	Epsilon (ppm)	778.2	2863.7	
	W	0.94	0.95	
	P	0.49	0.58	

exception is noted for the quantile method with data set B where the original fitted value for epsilon was negative (a physical impossibility) and thus automatically set to 0. The CML method does not estimate epsilon and the agreement between the sample mean and variance estimates and the fitted estimates are not as good as the prior two methods.

Table 4. Comparison of sample and fitted values.

Data ID		Sample	Quantile method	Method of moments	Conditional maximum likelihood (min = 0)
A (N = 33) (ppm)	Mean	0.278	No fit	No fit	0.282
	Standard dev	0.311			0.304
	Lambda	1.389			1.856
	Epsilon	0.011			0.000
B (N = 55) (mg/m^3)	Mean	135.5	138.14	135.5	136.35
	Standard dev	126.45	126.45	126.45	122.22
	Lambda	560.9	895.01	745.63	681.15
	Epsilon	7.703	0.000	4.06	0.000
C (N = 27) (ppm)	Mean	54.2	54.2	54.2	No fit
	Standard dev	11.74	11.74	11.74	
	Lambda	42.76	51.39	63.06	
	Epsilon	37.46	36.11	36.48	
D (N = 13) (ppm)	Mean	10461.5	10461.5	10461.5	No fit
	Standard dev	4884.93	4884.93	4884.93	
	Lambda	16600	102421.6	33138.3	
	Epsilon	5200	778.2	2863.7	

Figures 1–4 show the best fitting cumulative distribution along with the sample distribution for a visual comparison.

Discussion

The studies conducted here, although limited in scope, suggest that for an S_B population typical of occupational and environmental exposures, the quantile and method-of-moments fitting procedures *may* provide performance superior to that of the percentile methods, both in terms of accuracy and precision in parameter estimation, and also in the subsequent goodness of fit. These results are in general agreement with the more exhaustive simulation studies of Siekierski (1992). The S_B distribution offers an approach for estimating extreme values and this may be particularly useful in risk assessments and epidemiological investigations for determining background levels to which all members of the population are exposed.

Both quantile and method-of-moments procedures used here employ analytic expressions for the moments and numerical integration is not required. The method-of-moments involves calculation of the first four moments only, as the Jacobian matrix in the Newton solver (IMSL subroutine) is approximated with finite differences. The relative error tolerance used in calculating the moments was 10^{-20} and the tolerance for the iterative Newton solver was 10^{-4}. The quantile approach requires calculation of the first two moments to estimate the mean and variance of y in Eqs. (4) and (5) for determining epsilon and lambda.

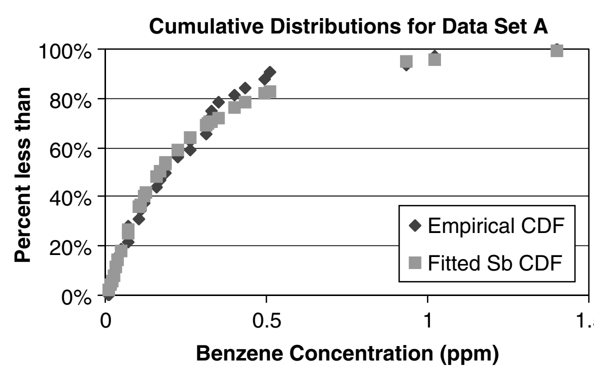

Figure 1. Cumulative distributions for the benzene data set A, the fitted distribution is obtained with the conditional maximum likelihood approach and *a priori* minimum of 0.

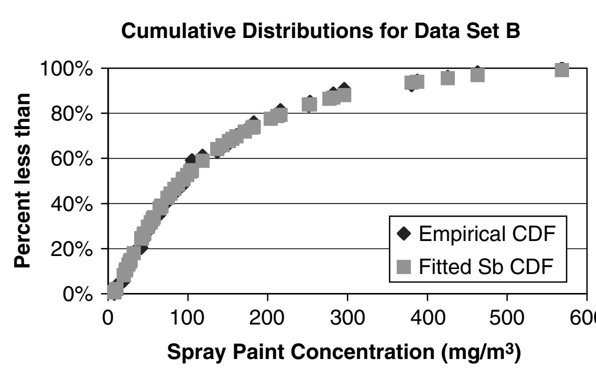

Figure 2. Cumulative distributions for the spray painting data set B, the fitted distribution is obtained with the method-of-moments approach.

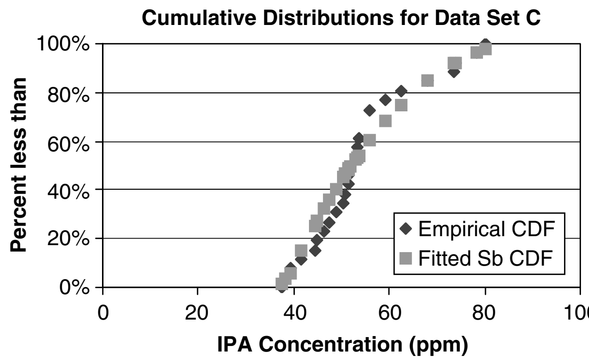

Figure 3. Cumulative distributions for the isopropyl alcohol data set C, the fitted distribution is obtained with the quantile approach.

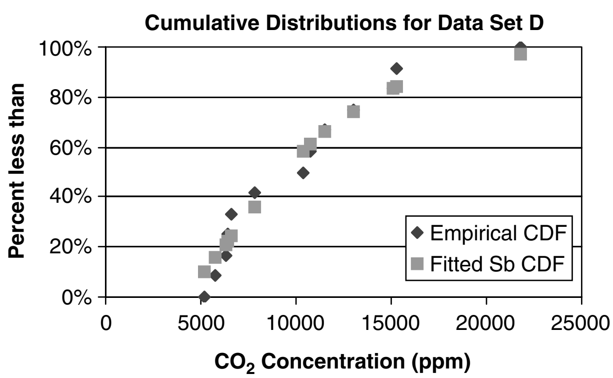

Figure 4. Cumulative distributions for the carbon dioxide data set D, the fitted distribution is obtained with the method-of-moments approach.

The Johnson S_B distribution is a flexible 4-parameter probability model well suited for characterizing variates bound by extreme values, or expressed as ratios. These attributes are appealing for characterizing human exposures to toxic contaminants and offer an alternative to traditional approaches. Estimation of background concentrations and/or maximal values may be useful as well as improved estimates of the mean and variance of exposures in epidemiological studies and risk assessments.

Difficulties in using the distribution are associated with mathematical complexity and lack of effective maximum likelihood methods when three or four parameters must be estimated. The methods performed well on three out of four real data sets, the one failure was well fit using a CML method with an *a priori* zero minimum. This is a reasonable approximation for many actual exposure data sets. The computer code is available upon email request from the author.

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Appendix A S_B equations:

The mean of y is (Johnson, 1949)

$$\mu(y) = \frac{\phi}{\psi} \tag{A.1}$$

where $\phi = \mathrm{A{-}B}$ and $\psi = CD$ and

$$A = \frac{1}{2\delta} + \frac{1}{2\delta}\sum_{n=1}^{\infty} \exp(-n^2/(2\delta^2))\cosh\left(\frac{n(1-2\delta\gamma}{2\delta^2}\right)\mathrm{sech}\left(\frac{n}{2\delta^2}\right) \tag{A.2}$$

$$B = 2\pi\delta\sum_{n=1}^{\infty} \exp\left(-\frac{1}{2}(2n-1)^2\pi^2\delta^2\right)\sin((2n-1)\pi\delta\gamma)\mathrm{cosech}\left((2n-1)\pi^{2\delta^2}\right) \tag{A.3}$$

$$C = 1 + 2\sum_{n=1}^{\infty} \exp(-2n^2\pi^2\delta^2)\cos(2n\pi\gamma\delta) \tag{A.4}$$

$$D = \sqrt{2\pi}\exp\left(\frac{\gamma^2}{2}\right) \tag{A.5}$$

The variance of y is

$$\sigma_y^2 = \mu_2' - \mu^2 \tag{A.6}$$

where μ'_2 is the second moment of y about the origin and

$$\mu_2' = \mu + \delta\frac{\partial\mu}{\partial\gamma} \tag{A.7}$$

Application of the chain rule to expression (A.7) and some algebraic simplification yields the following explicit expression for the variance of y:

$$\sigma_y^2 = \mu(1-\delta\gamma) + \frac{\delta}{\psi}\left[\frac{\partial A}{\partial\gamma} - \frac{\partial B}{\partial\gamma} - \mu\frac{\partial C}{\partial\gamma}D\right] - \mu^2 \tag{A.8}$$

The partial derivatives are

$$\frac{\partial A}{\partial\gamma} = -\frac{1}{\delta^2}\sum_{n=1}^{\infty} n\exp(-n^2/(2\delta^2)) \sinh\left[\frac{n(1-2\delta\gamma)}{2\delta^2}\right]\operatorname{sech}\left(\frac{n}{2\delta^2}\right) \tag{A.9}$$

$$\frac{\partial B}{\partial\gamma} = 2(\pi\delta)^2\sum_{n=1}^{\infty}(2n-1)\mathrm{e}^{\left(1/2(2\mathrm{n}-1)^2\pi^2\delta^2\right)} \cos((2n-1)\pi\delta\gamma)\operatorname{cosech}\left((2n-1)\pi^{2\delta^2}\right) \tag{A.10}$$

$$\frac{\partial C}{\partial\gamma} = -4\pi\delta\sum_{n=1}^{\infty} n\ \exp(-2n^2\pi^2\delta^2))\sin(2n\pi\gamma\delta) \tag{A.11}$$