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Note on the numerical evaluation of integrals of the form $\int_{-\infty}^{\infty} f(x) \phi(x) dx$, with particular reference to the determination of the expectation of a function of a normally distributed random variable.

Systems Evaluation Department

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ABSTRACT

A method is given for the rapid and accurate numerical integration of integrals of the form $\int_{-\infty}^{\infty} f(x) \phi(x) dx$, where $f(x)$ is "smooth." Tables are given for the special case $\phi(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-x^2/2\sigma^2}$.

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1. Introduction. This note is concerned with the numerical integration of integrals of the form $\int_{-\infty}^{\infty} f(x) \phi(x) dx$, where the function $f(x)$ is "smooth". It is often convenient to carry out such a numerical integration using values of the function $f(x)$ at equally spaced points. A particularly appropriate method would appear to be one which involves the exact integration of an integral obtained by replacing $f(x)$ by a smooth function interpolating the values of $f(x)$ at the equally spaced points. Such a function is given by the cardinal series associated with these values (for references to the literature on cardinal series, cf. J. M. Whittaker, Interpolation Theory).

The integral

$$I = \int_{-\infty}^{\infty} f(x) \phi(x) dx$$

is to be approximated in terms of the values, $\{f(k)\}$, ($k = 0, \pm 1, \pm 2, \dots$) of $f(x)$ at points with integral abscissas. The cardinal series, $f^*(x)$, associated with the values, $\{f(k)\}$, of $f(x)$ is given by:

$$f^*(x) = \sum_{k=-\infty}^{\infty} f(k) \frac{\sin \pi(x-k)}{\pi(x-k)}.$$

The integral I is approximated by

$$I^* = \int_{-\infty}^{\infty} f^*(x) \phi(x) dx,$$

$$I^* = \sum_{k=-\infty}^{\infty} f(k) \int_{-\infty}^{\infty} \frac{\sin \pi(x-k)}{\pi(x-k)} \phi(x) dx,$$

or

$$I^* = \sum_{k=-\infty}^{\infty} a_k f(k) \quad (1)$$

where

$$a_k = \int_{-\infty}^{\infty} \frac{\sin \pi(x-k)}{\pi(x-k)} \phi(x) dx. \quad (2)$$

Formula (1) has two important advantages, which are, of course, shared by other methods of numerical integration:

(A) The integral I^* is expressed as a linear combination of

the given values of f , and is thus particularly well-suited to calculation with a desk calculator.

(B) The coefficients, a_k , do not depend on the particular function, f .

2. The expectation of a function of a normally distributed random variable. Suppose it is desired to compute the expected value of a function, $f(x)$, of a normally distributed random variable x , and that coordinates have been chosen so that the mean of x is 0. The expectation of $f(x)$ is given by

$$I = \int_{-\infty}^{\infty} f(x) \varphi(x) dx,$$

where
$$\varphi(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-x^2/2\sigma^2}$$

and where σ is the standard deviation of x .

Let the function $f(x)$ be evaluated at equally spaced points, and let the distance between an adjacent pair of these points be chosen as unit. The integral I is then approximated by

$$I^* = \sum_{k=-\infty}^{\infty} a_k f(k), \quad (1)$$

where the coefficients a_k are tabulated for various σ in Table 1.

For $\sigma \geq 1$ an approximate formula for the coefficients a_k is

$$a_k \approx \frac{1}{\sqrt{2\pi}\sigma} e^{-k^2/2\sigma^2}. \quad (2)$$

The error for $\sigma = 1$ is 0.0006 when $k = 0$ and decreases as k increases. For $\sigma = 2$ the error in (2) is of the order of 10^{-10} and is smaller for larger σ . Thus we have the rather surprising result that for $\sigma \geq 1$ an integration scheme which is nearly exact for the cardinal series is obtained

simply by multiplying each value of the function $f(x)$ by the ordinate of the probability density function at the same point and adding the results. Whether or not this scheme is accurate for the integration of the function $f(x)$ itself depends, of course, on how close to the function $f(x)$ is its cardinal series. A rough check on the accuracy of interpolation by the cardinal series may be obtained by plotting the points $(k, f(k))$, joining them by a smooth curve, and comparing the resulting graph with the graph of $f(x)$.

In terms of arbitrary linear units, one concludes from the above observations that if the graph of $f(x)$ is sufficiently smooth, then accurate results are obtained by evaluating $f(x)$ at points at distance σ units apart and multiplying each such value by σ and by the corresponding ordinate of the probability density function:

$$\int_{-\infty}^{\infty} f(x) \phi(x) dx \approx \sum_{k=-\infty}^{\infty} \sigma f(k\sigma) \frac{1}{\sqrt{2\pi}\sigma} e^{- (k\sigma)^2 / 2\sigma^2},$$

or

$$\int_{-\infty}^{\infty} f(x) \phi(x) dx \approx \sum_{k=-\infty}^{\infty} f(k\sigma) \frac{1}{\sqrt{2\pi}} e^{- k^2 / 2}.$$

If the graph of the function $f(x)$ is not smooth enough that the cardinal series using values at points σ units apart represents the function accurately, then more closely spaced points may be used. If the function is evaluated at points at distance σ/n units apart, the approximate formula

$$\int_{-\infty}^{\infty} f(x) \phi(x) dx \approx \sum_{k=-\infty}^{\infty} f\left(\frac{k\sigma}{n}\right) \frac{1}{\sqrt{2\pi}n} e^{- k^2 / 2n^2}$$

may be used.

For a situation in which the integral I is to be computed for a fixed function f and for a number of different values of σ , it is desirable to have tables of the coefficients a_k for various σ . Such coefficients are given in Table I for $\sigma = 1/2, 1, 2, 3, 4, 5, 6, 8, 10, 12, 15, 20$. The distance between adjacent points at which f is evaluated is chosen as the linear unit in terms of which the standard deviation, σ , is measured.

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TABLE I - a_k

k	$\sigma=1/2$	$\sigma=1$	$\sigma=2$	$\sigma=3$	$\sigma=4$	$\sigma=5$	$\sigma=6$	$\sigma=8$	$\sigma=10$	$\sigma=12$	$\sigma=15$	$\sigma=20$
0	+.706	.398	.200	.132	.100	.080	.066	.050	.040	.034	.026	.020
± 1	+.160	.243	.176	.126	.097	.078	.066	.049	.040	.033	.026	.020
± 2	-.018	.054	.121	.106	.088	.074	.063	.048	.039	.033	.026	.020
± 3	+.008	.004	.065	.081	.075	.067	.059	.046	.038	.032	.026	.020
± 4	-.005	.000	.027	.055	.060	.058	.053	.044	.037	.031	.026	.020
± 5	+.003		.009	.033	.046	.048	.047	.041	.035	.030	.025	.019
± 6	-.002		.002	.018	.032	.039	.040	.038	.033	.029	.025	.019
± 7	+.002			.009	.022	.030	.034	.034	.031	.028	.024	.019
± 8	-.001			.004	.014	.022	.027	.030	.029	.027	.023	.018
± 9	+.001			.001	.008	.016	.022	.026	.027	.025	.022	.018
± 10	-.001			.001	.004	.011	.017	.023	.024	.024	.021	.018
± 11	+.001				.002	.007	.012	.019	.022	.022	.020	.017
± 12	-.001				.001	.004	.009	.016	.020	.020	.019	.017
± 13	.000				.001	.003	.006	.013	.017	.019	.018	.016
± 14						.002	.004	.011	.015	.017	.017	.016
± 15						.001	.003	.009	.013	.015	.016	.015
± 16							.002	.007	.011	.014	.015	.014
± 17							.001	.005	.010	.012	.015	.014
± 18							.001	.004	.008	.011	.013	.013
± 19							.001	.003	.007	.010	.012	.013
± 20								.003	.005	.008	.012	.012
± 21								.002	.004	.007	.010	.011
± 22								.002	.004	.006	.009	.011
± 23								.001	.003	.005	.008	.010
± 24								.001	.002	.005	.007	.010
± 25									.002	.004	.006	.009
± 26									.001	.003	.006	.009
± 27									.001	.003	.005	.008
± 28									.001	.002	.005	.007
± 29									.001	.002	.004	.007
± 30										.001	.004	.006
± 31										.001	.003	.006
± 32										.001	.003	.006
± 33										.001	.003	.005
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APPENDIX

Calculation of coefficients

A1. General. The coefficients a_k are given by the formula

$$a_k = \int_{-\infty}^{\infty} \frac{\sin \pi(x-k)}{\pi(x-k)} \phi(x) dx. \quad (A1)$$

It may also be convenient to use the expression derived below. We have

$$\begin{aligned} a_k &= \int_{-\infty}^{\infty} \phi(x) dx \cdot \frac{1}{\pi} \int_0^{\pi} \cos(x-k)t dt, \\ a_k &= \frac{1}{\pi} \int_0^{\pi} \cos kt dt \int_{-\infty}^{\infty} \phi(x) \cos xt dx \\ &\quad + \frac{1}{\pi} \int_0^{\pi} \sin kt dt \int_{-\infty}^{\infty} \phi(x) \sin xt dx. \end{aligned} \quad (A2)$$

If $\phi(x)$ is even, the second term on the right of equation (A2) vanishes, and the coefficient a_k is seen to be, except for a multiplicative constant, the k -th Fourier cosine coefficient of the cosine transform of $\phi(x)$:

$$a_k = \frac{1}{\pi} \int_0^{\pi} \cos kt dt \int_{-\infty}^{\infty} \phi(x) \cos xt dx. \quad (A3)$$

Similarly, if $\phi(x)$ is an odd function of x , we have

$$a_k = \frac{1}{\pi} \int_0^{\pi} \sin kt dt \int_{-\infty}^{\infty} \phi(x) \sin xt dx.$$

If $\phi(x)$ is even, then under conditions sufficient for the convergence of the Fourier series of the function $\int_{-\infty}^{\infty} \phi(x) \cos xt dx$ to the proper value, we have

$$\int_{-\infty}^{\infty} \phi(x) \cos xt dx = \sum_{k=-\infty}^{\infty} a_k \cos kt$$

for $|t| < \pi$. In this connection it is of interest to observe that on setting

$t = 0$ we have

$$\sum_{k=-\infty}^{\infty} a_k = \int_{-\infty}^{\infty} \varphi(x) dx.$$

Hence if $f(x)$ is identically constant, then the integrals I and I^* coincide, where

$$I = \int_{-\infty}^{\infty} f(x) \varphi(x) dx,$$

$$I^* = \int_{-\infty}^{\infty} f^*(x) \varphi(x) dx,$$

and
$$f^*(x) = \sum_{k=-\infty}^{\infty} f(k) \frac{\sin \pi(x-k)}{\pi(x-k)};$$

for
$$I^* = \sum_{k=-\infty}^{\infty} a_k f(k) = C \int_{-\infty}^{\infty} \varphi(x) dx$$

and
$$I = C \int_{-\infty}^{\infty} \varphi(x) dx$$

if $f(x)$ is the constant C . Thus the formula

$$I \approx \sum_{k=-\infty}^{\infty} a_k f(k) \tag{A4}$$

is exact when $f(x)$ is identically constant. Indeed, it can be shown that the cardinal series associated with values of a constant function is itself that constant; and since the formula is exact for every cardinal series, the above observation follows.

A2. The expectation of a function of a normally distributed random variable.

Let $\underline{x}$ be a normally distributed random variable with mean 0 and standard deviation σ . Its probability density function is

$$\varphi(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-x^2/2\sigma^2}$$

Let $f(\underline{x})$ be a function of the random variable $\underline{x}$. Its expectation is the integral

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$$I = \int_{-\infty}^{\infty} f(x) \varphi(x) dx = \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} f(x) e^{-x^2/2\sigma^2} dx.$$

Since $\varphi(x)$ is even, formula (A3) for the coefficient, a_k , is appropriate. We have

$$\begin{aligned} \int_{-\infty}^{\infty} \varphi(x) \cos xt dx &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} e^{-x^2/2\sigma^2} \cos xt dx \\ &= e^{-\sigma^2 t^2/2}. \end{aligned}$$

Formula (A3) then gives

$$a_k = \frac{1}{\pi} \int_0^{\pi} e^{-\sigma^2 t^2/2} \cos kt dt. \quad (A5)$$

The remainder of this section is devoted to the evaluation of this integral.

It is clear first of all that, for large σ ,

$$a_k \approx \frac{1}{\pi} \int_0^{\infty} e^{-\sigma^2 t^2/2} \cos kt dt,$$

$$a_k \approx \frac{1}{\sqrt{2\pi}\sigma} \left(\frac{\sigma}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\sigma^2 t^2/2} \cos kt dt \right),$$

and
$$a_k \approx \frac{1}{\sqrt{2\pi}\sigma} e^{-k^2/2\sigma^2}. \quad (A6)$$

The error involved in this approximation is not greater than

$$\begin{aligned} \frac{1}{\pi} \int_{\pi}^{\infty} e^{-\sigma^2 t^2/2} dt &= \frac{1}{\sigma} \sqrt{\frac{2}{\pi}} \left(\frac{\sigma}{\sqrt{2\pi}} \int_{\pi}^{\infty} e^{-\sigma^2 t^2/2} dt \right) \\ &= \frac{1}{\sigma} \sqrt{\frac{2}{\pi}} [1 - \Phi(\pi\sigma)], \end{aligned} \quad (A7)$$

where $\Phi(x)$ is the normal cumulative distribution function,

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-t^2/2} dt.$$

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For $\sigma = 1$ this upper bound on the error is 0.00064. For $\sigma = 2$ the error in formula (A6) is not greater than $6.78 (10^{-11})$. For larger σ , of course, the error is smaller.

For $k = 0$ and for arbitrary σ we have, from (A5),

$$a_0 = \frac{1}{\pi} \int_0^\pi e^{-\sigma^2 t^2/2} dt = \frac{1}{\sigma} \sqrt{\frac{2}{\pi}} \left(\frac{\sigma}{\sqrt{2\pi}} \int_0^\pi e^{-\sigma^2 t^2/2} dt \right),$$

$$a_0 = \frac{1}{\sigma} \sqrt{\frac{2}{\pi}} [\Phi(\pi\sigma) - 1/2], \quad (\text{A8})$$

where again $\Phi(x)$ is the normal cumulative distribution function.

It remains to develop methods for computing a_k from (A5) for $\sigma < 1$ and $k \geq 1$. On expanding the exponential in a power series, equation (A5) becomes

$$a_k = \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \left(\frac{\sigma^2}{2} \right)^j \cdot \frac{1}{\pi} \int_0^\pi t^{2j} \cos kt \, dt,$$

$$a_k = \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \left(\frac{\pi^2 \sigma^2}{2} \right)^j \int_0^1 u^{2j} \cos \pi k u \, du,$$

or

$$a_k = (-1)^k \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \left(\frac{\pi^2 \sigma^2}{2} \right)^j C_{k,j}, \quad (\text{A9})$$

where

$$C_{k,j} = (-1)^k \int_0^1 t^{2j} \cos \pi k t \, dt. \quad (\text{A10})$$

The constants $(-1)^k C_{k,j}$ are tabulated in Lowan and Laderman, Journal of Mathematics and Physics, 1943. For a situation in which these tables are not sufficiently extensive, the recursion formula derived below may be used. We have, from (A10), on integrating by parts,

$$C_{k,j} = (-1)^k \left\{ \left[t^{2j} \frac{\sin \pi k t}{\pi k} \right]_0^1 - \frac{2j}{\pi k} \int_0^1 t^{2j-1} \sin \pi k t \, dt \right\},$$

$$C_{k,j} = \frac{(-1)^{k+1} (2j)}{\pi k} \int_0^1 t^{2j-1} \sin \pi k t \, dt, \quad \text{for } j \geq 1, \quad k \geq 1.$$

A further integration by parts yields

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$$C_{k,j} = \frac{(-1)^{k+1}(2j)}{\pi k} \left\{ \left[\frac{-\cos \pi k t}{\pi k} (t^{2j-1}) \right]_0^1 + \frac{2j-1}{\pi k} \int_0^1 t^{2j-2} \cos \pi k t dt \right\},$$

$$C_{k,j} = \frac{2j}{(\pi k)^2} [1 - (2j-1) C_{k,j-1}] \quad (A11)$$

for $j \geq 1$, $k \geq 1$. Clearly

$$C_{k,0} = 0 \text{ if } k \geq 1,$$

$$C_{0,0} = 1.$$

The following alternative series expansion of a_k converges rapidly for small σ and large k . We have from (A5)

$$a_k = \frac{1}{\pi \sigma} \int_0^{\pi \sigma} e^{-u^2/2} \cos \frac{ku}{\sigma} du,$$

$$a_k = \frac{1}{\sigma} \sqrt{\frac{2}{\pi}} \int_0^{\pi \sigma} \psi(u) \cos \frac{ku}{\sigma} du,$$

where

$$\psi(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}.$$

Hence

$$\begin{aligned} \sigma \sqrt{\frac{\pi}{2}} a_k &= \int_0^{\pi \sigma} \psi(u) \cos \frac{ku}{\sigma} du \\ &= \left[\frac{\sigma}{k} \sin \frac{ku}{\sigma} \psi(u) \right]_0^{\pi \sigma} - \frac{\sigma}{k} \int_0^{\pi \sigma} \psi'(u) \sin \frac{ku}{\sigma} du \\ &= -\frac{\sigma}{k} \left\{ \left[-\frac{\sigma}{k} \cos \frac{ku}{\sigma} \psi'(u) \right]_0^{\pi \sigma} + \frac{\sigma}{k} \int_0^{\pi \sigma} \psi''(u) \cos \frac{ku}{\sigma} du \right\} \\ &= (-1)^k \frac{\sigma^2}{k^2} \psi'(\pi \sigma) - \frac{\sigma^2}{k^2} \int_0^{\pi \sigma} \psi''(u) \cos \frac{ku}{\sigma} du \\ &= (-1)^k \frac{\sigma^2}{k^2} \psi'(\pi \sigma) - (-1)^k \frac{\sigma^4}{k^4} \psi^{(3)}(\pi \sigma) + \dots \\ &= (-1)^k \frac{\sigma^2}{k^2} \sum_{r=0}^{\infty} (-1)^r \left(\frac{\sigma^2}{k^2} \right)^r \psi^{(2r+1)}(\pi \sigma), \end{aligned}$$

where $\psi^{(2r+1)}(\pi \sigma)$ is the $(2r+1)$ -st derivative of $\psi(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$

evaluated at $u = \pi\sigma$. Hence

$$a_k = (-1)^k \sqrt{\frac{2}{\pi}} \frac{\sigma}{k^2} \sum_{r=0}^{\infty} (-1)^r \left(\frac{\sigma}{k}\right)^{2r} \psi^{(2r+1)}(\pi\sigma). \quad (A12)$$

The Hermite polynomials, $H_j(x)$ are defined by

$$\psi^{(j)}(x) = (-1)^j H_j(x) \psi(x),$$

so that equation (A12) may be rewritten

$$a_k = (-1)^{k+1} \sqrt{\frac{2}{\pi}} \frac{\sigma}{k^2} \psi(\pi\sigma) \sum_{r=0}^{\infty} \left(\frac{\sigma}{k}\right)^{2r} H_{2r+1}(\pi\sigma). \quad (A13)$$

We have $H_0(x) = 1$, $H_1(x) = x$, $H_2(x) = x^2 - 1$, $H_3(x) = x^3 - 3x$,
 $H_4(x) = x^4 - 6x^2 + 3$, $H_5(x) = x^5 - 10x^3 + 15x$, $H_6(x) = x^6 - 15x^4 + 45x^2 - 15$.

Further $H_n(x)$ may be determined from the recurrence relation,

$$H_n(x) = x H_{n-1}(x) - H'_{n-1}(x).$$

For small k neither of the above series developments converges rapidly. On expanding the cosine in (A5) in a power series, we have

$$a_k = \sum_{j=0}^{\infty} (-1)^j \frac{k^{2j}}{(2j)!} \cdot \frac{1}{\pi} \int_0^{\pi} t^{2j} e^{-\sigma^2 t^2/2} dt.$$

Now
$$\frac{1}{\pi} \int_0^{\pi} t^{2j} e^{-\sigma^2 t^2/2} dt = \frac{1}{\pi \sigma^{2j+1}} \int_0^{\pi\sigma} u^{2j} e^{-u^2/2} du.$$

Let
$$A_j(x) = \frac{1}{\sqrt{2\pi}} \int_0^x u^{2j} e^{-u^2/2} du. \quad (A14)$$

Then
$$a_k = \sqrt{\frac{2}{\pi}} \frac{1}{\sigma} \sum_{j=0}^{\infty} \frac{(-1)^j}{(2j)!} \left(\frac{k}{\sigma}\right)^{2j} A_j(\pi\sigma). \quad (A15)$$

We have
$$A_j(x) = \frac{1}{\sqrt{2\pi}} [-u^{2j-1} e^{-u^2/2}]_0^x + \frac{2j-1}{\sqrt{2\pi}} \int_0^x u^{2j-2} e^{-u^2/2} du,$$

$$A_j(x) = -x^{2j-1} \psi(x) + (2j-1) A_{j-1}(x) \quad (j \geq 1), \quad (A16)$$

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where

$$\psi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$

We have

$$A_0(x) = \varphi(x) - 1/2,$$

where

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-t^2/2} dt,$$

$$A_1(x) = A_0(x) - x \psi(x),$$

$$A_2(x) = 3 A_0(x) - \psi(x) [x^3 + 3x],$$

$$A_3(x) = 15 A_0(x) - \psi(x) [x^5 + 5x^3 + 15x],$$

$$A_4(x) = 105 A_0(x) - \psi(x) [x^7 + 7x^5 + 35x^3 + 105x].$$

Further $A_j(x)$ can be determined from the recurrence relation (A16).

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