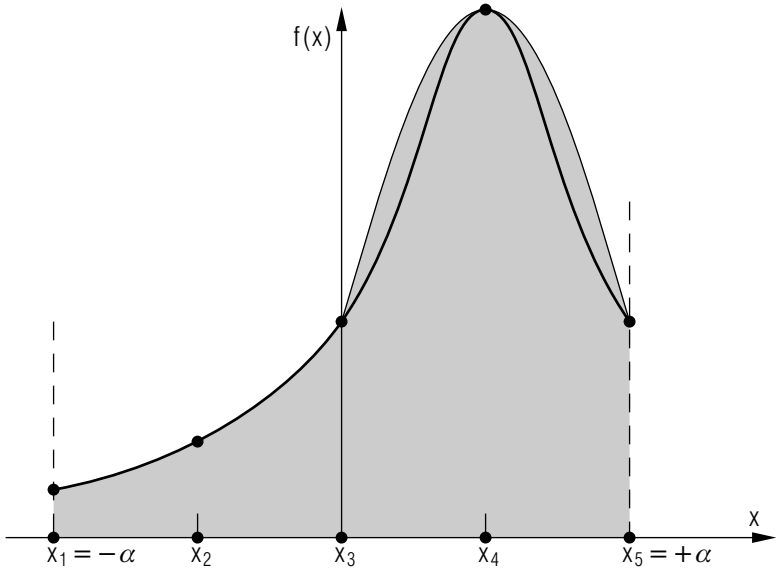
PHYSNET

MISN-0-349

NUMERICAL INTEGRATION



Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

NUMERICAL INTEGRATION

by

Robert Ehrlich
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Title: **Numerical Integration**

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Version: 3/8/2002 Evaluation: Stage 0

Length: 2 hr; 20 pages

Input Skills:

1. Vocabulary: linear charge density (MISN-0-147).
2. Write (or modify) and run programs that utilize advanced programming features such as type declarations and loop in FORTRAN (MISN-0-347) or in BASIC.
3. Express the net electric potential at some point in space as an integral over a continuous charge distribution (MISN-0-147).

Output Skills (Knowledge):

K1. Vocabulary: interpolating polynomial, Simpson's rule, finite sum rule, Simpson's 3/8 rule, trapezoidal rule, weighting coefficients.

K2. Discuss the relative merits of the various interpolating polynomials from the point of view of the accuracy of the approximation and the amount of computer time required.

Output Skills (Project):

P1. Compute and graph the error for the approximate electric potential resulting from a numerical integration using interpolating polynomials of zeroth order (finite sum rule), first order (trapexoidal rule), and second order (Simpson's rule).

P2. Determine the convergence of the approximate electric potential resulting from a numerical integration for third order interpolating polynomial (Simpson's 3/8 rule) and fourth order interpolating polynomial (Bode's rule).

P3. Calculate and explain the convergence and the dependence of the errors on k, when calculating the approximate electric potential for a non-uniform charge density of the form $\lambda(x) = cos(k\pi x)$ via second, third and fourth order polynomials.

External Resources (Required):

1. A computer with BASIC or FORTRAN.

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1. Numerical Integration Algorithms

1a. Introduction. In this module algorithms for numerical integration are developed. The definition of the integral of a function $f(x)$ is such that the integral

$$I = \int_a^b f(x)\,dx\,.$$

can be numerically approximated by the finite sum:

$$I_N = \sum_{j=1}^{N} f(x_j)\Delta x \tag{1}$$

where

$$\Delta x = \frac{(b-a)}{N-1}.$$

The accuracy of the approximation obviously increases as an N is increased, in view of the definition:

$$\lim_{N\to\infty} I_N.$$

This procedure is graphically illustrated in Fig.1. Including more terms in the sum for I_N invariably means more computer time, therefore we wish to find methods of obtaining better approximation to an integral that do not increase N. One method uses "weighting coefficients" $c_1, c_2, ...c_N$ in the sum:

$$I_N = \sum_{j=1}^{N} c_j f(x_j)\Delta x \tag{2}$$

The usefulness of this method hinges on the fact that the weighting coefficients do not depend on the particular function $f(x)$, but can be found using the appropriate interpolating polonomial.

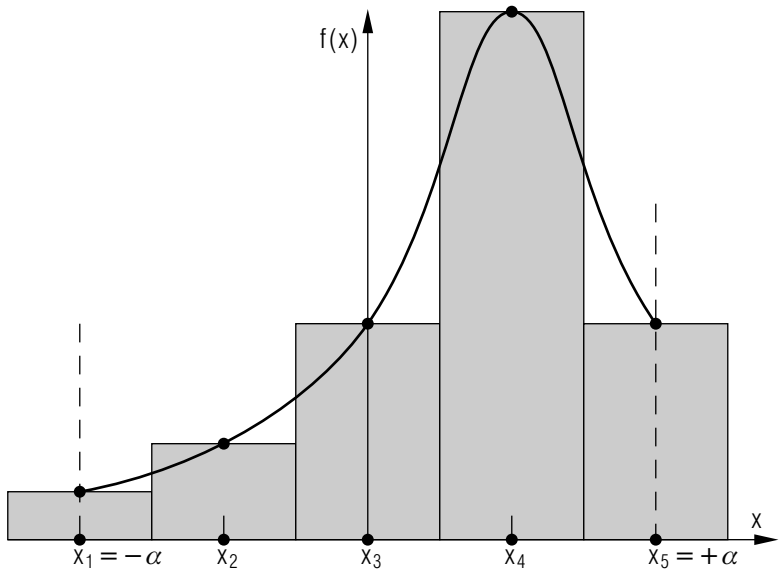

Figure 1. Approximation of the integral by a finite sum.

1b. Trapezoidal Rule. The simplest interpolation method is to assume the function $f(x)$ varies linearly in between each pair of consecutive points x_j and x_{j+1}. In this case we are geometrically approximating the area under the function $f(x)$ by a series of trapezoids rather than a series of rectangles (see Fig.2). The area of consecutive trapezoids are given by

$$A_1 = \frac{1}{2}[f(x_1) + f(x_2)]\Delta x$$

$$A_2 = \frac{1}{2}[f(x_2) + f(x_3)]\Delta x$$

$$\vdots$$

$$A_{N-1} = \frac{1}{2}[f(x_{N-1}) + f(x_N)]\Delta x$$

For the total area we, therefore, have

$$A = \frac{1}{2}f(x_1) + \sum_{j=2}^{N-1} f(x_j)\Delta x + \frac{1}{2}f(x_N)$$

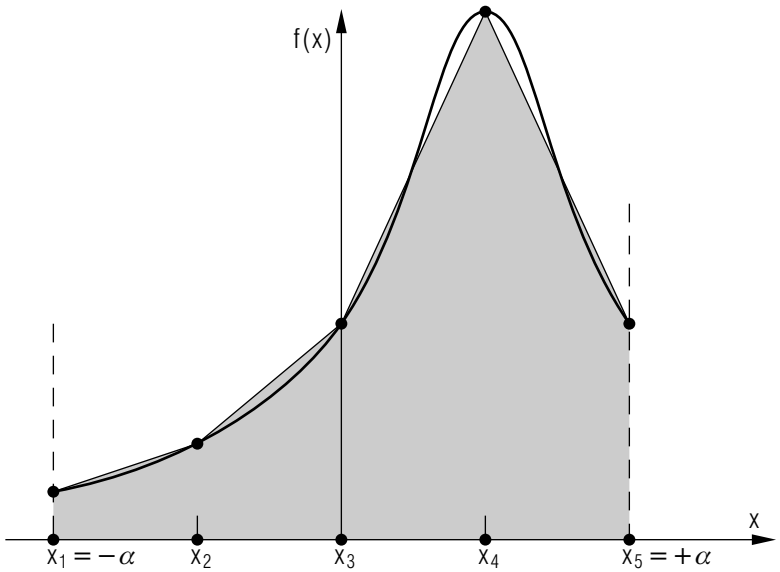

Figure 2. Trapezoidal approximation to the integral.

which can be expressed in the form of Eq.(2) provided: $c_1 = c_N = 1/2$, and $c_j = 1$ otherwise. In order to find the weighting coefficients $c_1, c_2, ...c_N$ corresponding to other higher order approximations, we need to use curves other than straight lines which pass through the points $x_1, x_2, ...x_N$ at which the function $f(x)$ is defined.

1c. Interpolating Polonomials. Given a set of N distinct points in a plane: (x_1, y_1), $...(x_N, y_N)$, a unique polonomial of $(N-1)^{\text{th}}$ order can be made to pass through the points. For example, a unique second order polonomial (parabola) passes through any three points (x_1, y_1), (x_2, y_2) and (x_3, y_3). It is surprisingly easy to write the equation of the interpolating polonomials. In the case $N = 3$, for example, the proper equation is:

$$y = f(x) = Ay_1 + By_2 + Cy_3 \tag{3}$$

where

$$A \equiv A(x) = (x - x_2)(x - x_3)/\Delta x^2,$$

$$B \equiv B(x) = (x - x_1)(x - x_3)/\Delta x^2,$$

$$C \equiv C(x) = (x - x_1)(x - x_2)/\Delta x^2.$$

We can easily check that this is the correct equation by observing that:

(1) The coefficients A, B, C are quadratic functions of x, so that $y(x)$ is, in fact, a second order polonomial.

(2) When $x = x_1$, we have $A = 1$ and $B = C = 0$, so that $y = y_1$.

(3) When $x = x_2$, we have $B = 1$ and $A = C = 0$, so that $y = y$.

(4) When $x = x_3$, we have $C = 1$, and $A = B = 0$, so that $y = y$.

Similar interpolating polonomials can be written down by inspection for any order N. *Help: [S-1]*

1d. Simpson's Rule. The geometrical basis of Simpson's rule is that a parabola is passed through each three consecutive points at which the function $f(x)$ is defined. The area under this series of parabolas approximates that under the function $f(x)$. The area under the first parabola can be easily obtained by integrating Eq.(3) from x_1 to x_3. The result for the area under the first parabola is:

$$A_1 = \frac{\Delta x}{3}(y_1 + 4y_2 + y_3),$$

where $\Delta x = x_2 - x_1 = x_3 - x_2$. Similarly, the area under the parabola passing through the next three points in sequence is given by:

$$A_2 = \frac{\Delta x}{3}(y_3 + 4y_4 + y_5)$$

and so on for any remaining parabolas. The total area under all the parabolas may be easily seen to be given by:

$$A = \frac{\Delta x}{3}(y_1 + 4y_2 + 2y_3 + 4y_4 + ... + 4y_{N-1} + y_N)$$

Recalling that y = f(x), we may easily express this as another special case of Eq.(2):

$$I_N = \sum_{j=1}^{N} c_j f(x)\Delta x$$

where we now have: $c_1 = c_N = 1/3$, and otherwise $c_j = 4/3$ for j even, or $c_j = 2/3$ for j odd. The use of Simpson's rule requires that N be an odd number, since otherwise we cannot cover all N points using a series of parabolas each of which connects three points.

1e. Higher Order Approximations. The procedure for carrying out still higher order approximations to an integral is the same as that which has already been used for the trapezoidal rule and Simpson's rule. For example, suppose that we wish to approximate the function $f(x)$ by a series of third order polonomials. In that case, we first write down the form of the appropriate interpolating polonomial and integrate it to obtain the coefficients c_1. These coefficients which have been tabulated in the fourth row of Table 1 are the same for any function $f(x)$ that we wish to integrate. The integral can then be found directly from Eq.(2). In order to use a series of third order polonomials to approximate $f(x)$ there must be at least $N = 4$ points, and furthermore $N - 1$ must be divisible by 3. In Table 1 we also show the proper coefficients c_j to use for polonomials of order 4 as well. In this case $N - 1$ must be divisible by 4, so that an even number of 4^{th} order polonomials can cover all the points. In the next section we consider a specific physical problem to which we shall apply these numerical integration methods.

Table 1. Values of coefficients appearing in m^{th} order interpolating polynomial

m	0	1	2	3	4
Name	finite rule	trapazoidal rule	Simpson's rule	Simpson's 3/8 rule	Bode's rule
Minimum n allowed	1	2	3	4	5
Other restrictions on n	none	none	$n = 2k + 1^*$	$n = 3k + 1^*$	$n = 4k + 1^*$
c_1	1	1/2	1/3	3/8	14/45
c_2	1	1	4/3	9/8	64/45
c_3	1	1	2/3	9/8	24/45
c_4	1	1	4/3	3/4	64/45
c_5	1	1	2/3	9/8	28/45
c_6	1	1	4/3	9/8	64/45
c_7	1	1	2/3	3/4	24/45
c_8	1	1	4/3	9/8	64/45
c_9	1	1	2/3	9/8	28/45
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
c_{N-4}	1	1	2/3	9/8	28/45
c_{N-3}	1	1	4/3	3/4	64/45
c_{N-2}	1	1	2/3	9/8	24/45
c_{N-1}	1	1	4/3	9/8	64/45
c_N	1	1/2	1/3	3/8	14/45

* k can be any positive integer

2. Potential for a Charged Thin Wire

2a. Introduction. In order to calculate the potential for a charged thin wire, we can assume that the net charge on the wire consists of a row of closely spaced point charges. We can easily calculate the potential V at any point (x, y) in a plane containing the wire using Eq.(4). In practice, however, the number of excess electrons on a charged wire is usually so large that we can regard the charge on the wire as continuously distributed along its length, and speak of a line of charge. Mathematically, what we

have done is to replace the finite sum appearing in Eq.(4) by an integral. Suppose each of the N point charges in the row has a value Δq, such that the total charge of all the N charges is a constant q, independent of N. Then, by definition of a definite integral, the finite sum

$$V = \sum_{j=1}^{N} \frac{\Delta q}{r_j} \tag{4}$$

approaches the integral

$$V = \int \frac{dq}{r} \tag{5}$$

in the limit as N becomes infinite and Δq tends to zero.[1]

2b. Transforming the Integral. Let us put the integrand in Eq.(5) in a form which can be directly evaluated. We choose the x-axis to lie along the wire, and we assume that the wire extends from $x = -a$ to $x = +a$. The charge dq contained within a given length of wire dx is given by

$$dq = \lambda(x)dx \tag{6}$$

where $\lambda(x)$ is some function which gives the linear charge density at position x. The factor r in Eq.(5) is the distance from a point $(x, 0)$ on the wire to some point (x_0, y_0), at which we wish to find the potential (see Fig.3), and r is given by

$$r = \sqrt{(x - x_0)^2 + y_0^2} \tag{7}$$

Substitution of Eqs.(6) and (7) into (5) yields

$$V(x_0, y_0) = \int_{-\alpha}^{+\alpha} \frac{\lambda(x)}{\sqrt{(x - x_0)^2 + y_0^2}} dx. \tag{8}$$

[1]For a deeper discussion of this transition from discrete sums to integrals, see "Electrostatic Potential Due to a Continuous Charge Distribution," (MISN-0-147).

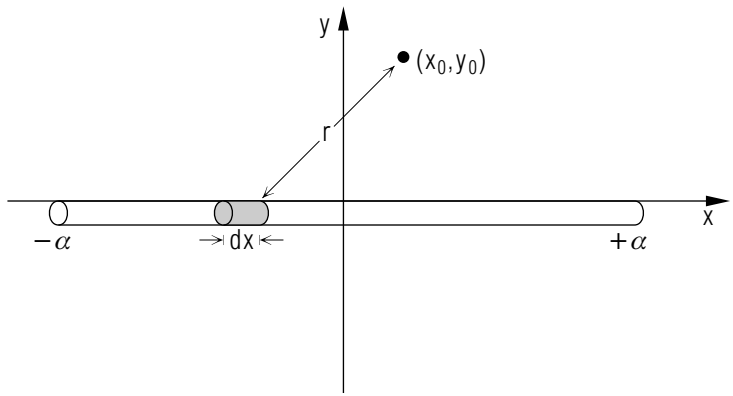

Figure 3. A charged thin wire.

2c. Exact Solution for a Special Case. For the case of a wire that has charge uniformly distributed along its length, the function $\lambda(x)$ is simply a constant λ_0. In this case, the integral in Eq.(8) can be directly evaluated, to give

$$V(x_0, y_0) = \lambda_0 \, \ell n \left\{ \frac{\sqrt{(x_0 - \alpha)^2 + y_0^2} - (x_0 - \alpha)}{\sqrt{(x_0 + \alpha)^2 + y_0^2} - (x_0 + \alpha)} \right\} \tag{9}$$

There are only a few special cases [such as $\lambda(x)$ constant] for which the integral in Eq.(8) can be directly evaluated. In other cases, we must use approximate numerical integration techniques, such as those discussed in the previous section, to calculate the integral. Knowing the exact solution for $\lambda(x)$ constant serves as a valuable check on the accuracy of the approximate numerical methods.

3. Computer Implementation

3a. Input. The program first reads numerical values for the parameters `N`, `A`, `XO`, and `YO` where

`N` $= n$	the number of terms in the sum
`A` $= \alpha$	half the length of the wire, which extends from $-\alpha$ to $+\alpha$
`XO` $= x_0$ `YO` $= y_0$	coordinates at which the potential is to be found.

Three sample sets of data include:

	N	A	XO	YO
1st	3.0	1.0	0.0	1.0
2nd	10.0	1.0	0.0	1.0
3rd	100.0	1.0	0.0	1.0

3b. Output. The program calculates the exact potential (V_1) and three approximate potentials based on: The finite sum (V_2), the trapezoidal rule (V_3) and Simpson's rule (V_4) according to Eq.(2). The exact result only holds for the special case $\lambda(x) = \lambda_0 = 1$. The output corresponding to the sample input is as follows:

N = 3.00000	A = 1.00000	XO = .00000	YO = 1.00000
V1 = 1.76275	V2 = 2.41422	V3 = 1.70711	V4 = 1.80474
N = 11.00000	A = 1.00000	XO = .00000	YO = 1.00000
V1 = 1.76275	V2 = 1.90181	V3 = 1.76039	V4 = 1.76275
N = 101.00000	A = 1.00000	XO = .00000	YO = 1.00000
V1 = 1.76275	V2 = 1.77687	V3 = 1.76273	V4 = 1.76275

Note that if N is an even number, as in the second and third cases, the program actually uses the next higher odd integer. The reason for this is that Simpson's rule can only be used with odd values of N, and we want to compute V_1, V_2, V_3, and V_4 all for the same value of N. Then we can compare the various approximation methods at the same value of N.

4. Procedures

4a. Original Program - Dependence on N. Run the program using these values of the input parameters:

A	XO	YO
1.0	0.0	1.0

and N = 3, 11, 31, 101, 301. For each of the three approximations: finite sum (V_2), trapezoidal (V_3), and Simpson's rule (V_4), compute the error which is the difference from the exact solution (V_1). Make a graph of the error as a function of log N for each of the three approximations. How do the three rates of convergence compare? How did the program execution time depend on N.

4b. Original Program - Dependence on YO. Run the program using these values of the input parameters:

N	A	XO
11	1.0	0.0

and YO = 1.0, 3.0, 10.0, 20.0, 30.0, and 100. Compute the errors for each of the three approximations as in the procedure in paragraph 4a, and plot a graph of the errors as a function of log YO in each case. Explain why the errors are found to decrease with increasing YO. Hint: How does the shape of the integrand change as YO is increased?

4c. Modified Program - Higher Order Approximations. Modify the program so that it includes the third and fourth order interpolating polonomials for the numerical integration. *Help: [S-1]* You will need to explicitly calculate the coefficients listed in the fourth and fifth rows of Table 1 in terms of the running index J. Run the modified program and follow the procedure in paragraph 4a to see how rapidly these two higher order approximations converge with N.

4d. Modified Program - Non-Uniform Charge Distribution. Modify the program so that it calculates the potential due to a charged wire having a nonuniform charge density. One interesting function is $\lambda(x) = \cos(k\pi x)$ which changes sign $k-1$ times along the length of the wire. You should modify the program so that the parameter k can be read in along with the other input parameters: N, A, XO, and YO. Note, that in this case the exact solution cannot be obtained, so that the value calculated for V_1 is meaningless. Choose the input parameters as follows:

N	A	XO	YO
101	1.0	0.0	1.0

and $k = 1, 3, 10, 30, 100$. If there is very little difference between the three approximations V_2, V_3 and V_4 then all of these are very good approximations and they are close to the exact solution. The best approximate of the three will be the one that is highest order (V_4). The differences $V_2 - V_4$ and $V_3 - V_4$ are one measure of the error of V_2 (finite sum) and V_3(trapezoidal) approximations. How are these errors found to depend on k? Explain this result.

Acknowledgments

Preparation of this module was supported in part by the National Science Foundation, Division of Science Education Development and Research, through Grant #SED 74-20088 to Michigan State University.

Glossary

- **interpolating polynomial:**: a polynomial of order N which exactly passes through $(N + 1)$ given points, useful for interpolating between the points.
- **trapezoidal rule:**: the integral is a multiplier times the sum of the integrand values at variable-of-integration points that are evenly spaced between the limits of integration, except that the values at each of the end points has a relative weight that is 1/2 the weight of each of the other values. The multiplier is the distance between successive values of the variable of integration.
- **Simpson's rule:**: a rule for finding a definite integral by: (i) breaking the variable of integration into $(1+2n)$ evenly spaced points that begin and end with the limits of integration, where n is any positive integer; (ii) summing the values of the integrand at those points, using weighting coefficients proportional to $(1, 4, 2, 4, 2, ..., 2, 4, 2, 4, 1)$; and (iii) multiplying the sum by the distance of integration and dividing by the sum of the weighting coefficients.
- **Finite sum rule:**: this rule is similar to Simpson's rule (see above) except that: (i) the variable of integration can be broken up into any number of equal intervals; (ii) the integrand is evaluated at the midpoints of the intervals; and (iii) the weighting coefficients proportional to $(1, 1, 1, 1...1, 1, 1, 1)$.
- **Simpson's 3/8 rule:**: similar to Simpson's rule (see above) except that: (i) $(1 + 3n)$ evenly spaced points; (ii) the weighting coefficients are proportional to $(3, 9, 9, 6, 9, 9, 6, ..., 6, 9, 9, 3)$.
- **Weighting coefficients in integration rules:**: a term which always refers to numbers that multiply the numerical values of the integrand being summed to obtain an integral. Some authors multiply all of the coefficients (for a given rule) by some constant factor and some authors show them as including the point-to-point integration interval. The wise user determines what constant multiplier to use with any particular set of coefficients by using them on a constant integrand.

A. Fortran, Basic, C++ Programs

All programs are at

`http://www.physnet.org/home/modules/support_programs`

which can be navigated to from the home page at

`http://www.physnet.org`

by following the links: → `modules` → `support programs`, where the programs are:

`m349p1f.for`, Fortran;
`m349p1b.bas`, Basic;
`m349p1c.cpp`, C++;
`lib351.h`, C++;

SPECIAL ASSISTANCE SUPPLEMENT

S-1 *(from TX-4e)*

For the third order plonomial which passes through the four points (x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), the correct form is:

$$y(x) = Ay_1 + By_2 + Cy_3 + Dy_4$$

where:

$$A = (x - x_2)(x - x_3)(x - x_4)/\Delta x^3$$
$$B = (x - x_1)(x - x_3)(x - x_4)/\Delta x^3$$
$$C = (x - x_1)(x - x_2)(x - x_3)/\Delta x^3$$
$$D = (x - x_1)(x - x_2)(x - x_3)/\Delta x^3$$

MODEL EXAM

1-2. See Output Skills K1-K2 in this module's *ID Sheet*.

Examinee:
On your computer output sheet(s):

(i) Mark page numbers in the upper right corners of all sheets.

(ii) Label all output, including all axes on all graphs.

On your Exam Answer Sheet(s), for each of the following parts of items (below this box), show:

(i) a reference to your annotated output; and

(ii) a blank area for grader comments.

When finished, staple together your sheets as usual, but include the original of your annotated output sheets just behind the Exam Answer Sheet.

3. Submit your annotated computer output that shows your runs of the original program in the module, pointing out how the errors in the three lowest order approximations for the integrals depend on:
   a. the number of intervals, `N`, and
   b. the y-coordinate of the point at which the potential is found.
4. Submit your annotated computer output that shows how the higher order approximations to the integral depend on `N`, the number of terms in the sum.
5. Submit your annotated computer output that shows results and relevant discussion of them for the modified program that calculates the potential at a point in space due to a charged wire with a linear charge distribution given by $\lambda(x) = cos(k\pi x)$.

INSTRUCTIONS TO GRADER

If the student has submitted copies rather than originals of the computer output, state that on the exam answer sheet and **immediately stop grading the exam and give it a grade of zero.**