

As x decreases, $K_\nu(x)$ increases rapidly while $I_\nu(x)$ decreases rapidly. Therefore, the error introduced by the truncation, decreases in the case of $K_\nu(x)$, and increases in the case of $I_\nu(x)$. This difficulty is avoided by calculating ρ . That is, at $x = 2$, e.g., where $K_\nu(x)$ is still accurately given by the solution of the differential equations, equations (17) and (18)

$$(24) \quad \rho = \frac{\tilde{I}_\nu(x) - I_\nu(x)}{K_\nu(x)}.$$

At $x = 2$, $I_\nu(x)$ is easily obtained by standard methods, e.g. the defining series, or integral representation.

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1. W. E. MILNE, "The numerical determination of characteristic numbers," *Phys. Rev.*, v. 35, 1930, p. 863-867.

2. HAROLD JEFFREYS, "On certain approximate solutions of linear differential equations of the second order," *London Math. Soc., Proc.*, v. 23, 1923, p. 428-436.

The mathematical method first given by Jeffreys was independently derived in connection with an important physical problem by

a. G. WENTZEL, "Eine Verallgemeinerung der Quantenbedingungen für die Zwecke der Wellenmechanik," *Zeits. f. Physik*, v. 38, 1926, p. 518-529.

b. H. A. KRAMERS, "Wellenmechanik und halbzahlige Quantisierung," *Zeits. f. Physik*, v. 39, 1926, p. 828-840.

c. L. BRILLOUIN, "La mécanique ondulatoire de Schrödinger; une méthode générale de résolution par approximations successives," *Comptes Rendus*, v. 183, 1926, p. 24-26.

d. L. BRILLOUIN, "Remarques sur la mécanique ondulatoire," *J. de Physique*, v. 7, 1926, p. 353-368, and is commonly referred to as the JWKB approximation.

Numerical Experiments in Potential Theory Using the Nehari Estimates

By U. W. Hochstrasser

1. Introduction. It is well known that the Dirichlet problem can be solved by using a set of harmonic functions which are orthogonal over the boundary [7]. Prior to the availability of high speed computers, however, the method was not frequently used since generating sets of orthogonal functions by hand computations is very laborious. With the advent of high speed computers interest in the method has been renewed and several papers have appeared recently [1, 2, 3].

In using the method, the numerical analyst is particularly interested in estimates of the error committed by replacing infinite orthogonal expansions by finite ones. Nehari [1] recently has given such estimates for a number of Dirichlet problems. The purpose of the present paper is to report the results of some numerical experiments which were designed to investigate how close these estimates come to the actual errors in certain particular examples. An existing computer program [4] was used for the orthogonalization of a given set of vectors on the SEAC com-

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puter at the National Bureau of Standards. Several boundary value problems, each involving the same irregular pentagon, were solved. For two of these problems the exact solution is known so that one can compare the exact errors with the estimates. In all cases the number of orthogonal harmonic functions used to approximate the solution was varied. The effect of using a sophisticated choice of the harmonic functions was also studied.

2. Dirichlet problems for an irregular pentagon. In the experiments an irregular pentagon inscribable in a circle was used in all the cases as the region on which the Dirichlet problem was defined (see Figure 1).

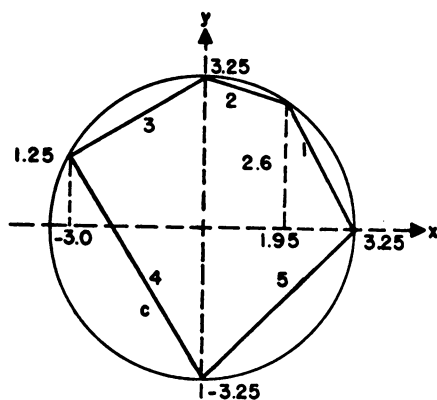


FIG. 1

For this region the following Dirichlet problems were considered:

(a) The boundary values are given by

$$U(x, y) = \operatorname{Re} (\cos z) = \operatorname{Re} \cos (x + iy) = \cos x \cosh y.$$

(b) The boundary values are given by

$$U(x, y) = \operatorname{Re} \frac{1}{z + 4} = \frac{x + 4}{(x + 4)^2 + y^2}.$$

(c) The boundary values are equal to one on one side and zero on all the others. (The solutions of these problems are the harmonic measures for the sides.)

The solution of the first Dirichlet problem changes sign in the interior and on the boundary of the region. In the second case the solution is always positive on the whole region. The set of functions which were used to approximate the solution in the cases *a* and *b* consisted of harmonic polynomials obtained by orthonormalizing $1, \operatorname{Re} z, \operatorname{Im} z, \operatorname{Re} z^2, \operatorname{Im} z^2, \dots$ on the region. It was expected that with a few functions one would obtain a better approximation in the second case than in the first.

In order to find approximate values for the harmonic measures of the sides of the pentagon one can start from the harmonic measure of the circumscribed circle. Let the segment 2α be that part of the circumference of this circle which is cut out by the side of the pentagon with boundary values equal to 1. Then the harmonic measure u_0 which has the value 1 on the segment 2α and 0 on the rest of the circumference

is given by

$$u_0 = \frac{\varphi - \alpha}{\pi - 2\alpha}$$

(see Figure 2)

$$\varphi = \arccos \left[\frac{(x - x_2)(x - x_1) + (y - y_2)(y - y_1)}{\sqrt{[(x - x_1)^2 + (y - y_1)^2][(x - x_2)^2 + (y - y_2)^2]}} \right]$$

$$\alpha = \frac{1}{2} \arccos \left[\frac{x_1 x_2 + y_1 y_2}{x_1^2 + y_1^2} \right]$$

where φ is the angle belonging to any point in the region and (x_1, y_1) , (x_2, y_2) are the coordinates of the end points of that side of the pentagon with boundary values

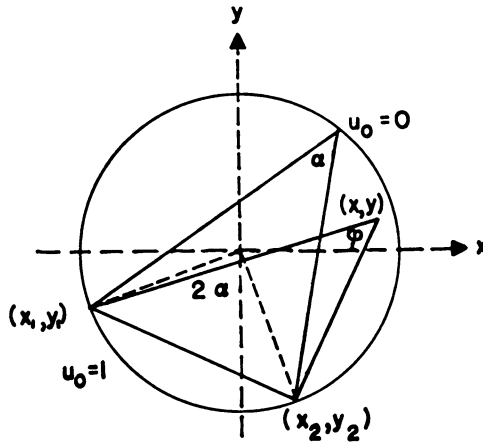


FIG. 2

equal to 1. In addition to these harmonic measures the harmonic polynomials $1, \operatorname{Re} z, \operatorname{Im} z, \operatorname{Re} z^2, \operatorname{Im} z^2, \dots$ were used for obtaining the set of approximating functions. These sets were orthonormalized with respect to the inner product

$$(f, g) = \int_c f(x, y)g(x, y)ds, \quad ds^2 = dx^2 + dy^2$$

where the integration is along the boundary c of the region.

If n functions $1, \operatorname{Re} z, \operatorname{Im} z, \operatorname{Re}(z^2), \operatorname{Im}(z^2), \dots$ are used as basic set one obtains after orthonormalization a system of n orthonormal harmonic polynomials $u_\nu(x, y)$. The approximate solution of the Dirichlet problem is given then by the sum

$$u(x, y) = \sum_{\nu=1}^n \left[\int_c U(X, Y)u_\nu(X, Y)dS \right] u_\nu(x, y), \quad (dS^2 = dX^2 + dY^2).$$

For the numerical computations the contour integrals appearing in these computations must be replaced by an integration formula involving finite sums. Since the contour consists of straight lines, splitting the integral into five integrals corresponding to the five sides of the contour was suggested.

For their evaluation an eight point Gaussian-type integration rule was chosen involving the end points of the interval of integration as given by Radau [5].

This rule is exact for polynomials up to degree 13. It corresponds therefore to a seven point ordinary Gaussian integration rule. Since it involves the endpoints, the computational work for the eight point Radau rule and the seven point Gaussian rule is, however, the same for a closed contour. Radau's formula has the added convenience of using the corner points of the pentagon. Thus the contour integral is replaced by a sum over 35 products of the form

$$\int_c G(x, y) ds \sim \sum_{i=1}^{i=5} \sum_{j=1}^{j=7} w_{ij} G(A_j x_i + (1 - A_j) x_{i-1}, A_j y_i + (1 - A_j) y_{i-1})$$

where (x_i, y_i) are the coordinates of the vertices of the pentagon

$$(x_0 = x_5, y_0 = y_5)$$

and the weights w_{ij} as well as the coefficients A_j are given by the integration rule

$$w_{ij} = \frac{1}{2} \sqrt{(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2} H_j \quad j = 2, 3, \dots, 7, i = 1, 2, \dots, 5$$

$$w_{i1} = \frac{1}{2} \{ \sqrt{(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2} + \sqrt{(x_{i-1} - x_{i-2})^2 + (y_{i-1} - y_{i-2})^2} \} H_1. \quad (x_{-1} = x_4, y_{-1} = y_4)$$

<i>j</i>	1	2	3	4	5	6	7
<i>H_j</i>	.03571 428	.21070 422	.34112 270	.41245 880	= <i>H₄</i>	= <i>H₃</i>	= <i>H₂</i>
<i>A_j</i>	0	.06412 9925	.20414 991	.39535 039	1 - <i>A₄</i>	1 - <i>A₃</i>	1 - <i>A₂</i>

The orthonormalization is carried out by the Gram-Schmidt process: If f_i is a set of n vectors with N components then a system of orthonormal vectors u_i with components u_{ik} , is found by the formulas

$$\begin{aligned} u_1 &= a_{11} f_1 \\ u_2 &= a_{21} f_1 + a_{22} f_2 \\ &\vdots \\ &\vdots \\ u_n &= a_{n1} f_1 + a_{n2} f_2 + \dots + a_{nn-1} f_{n-1} + a_{nn} f_n \end{aligned}$$

where the a_{ij} are determined by the orthogonality and normalization condition

$$\begin{aligned} (u_i, u_j) &= \delta_{ij} = 1; i = j & i, j &= 1, 2, \dots, n. \\ &= 0; i \neq j \end{aligned}$$

Since in the continuous case the orthonormalization is with respect to the contour integral $\int_c f(x, y) u(x, y) ds$, the inner product is defined by

$$(f_i, u_j) = \sum_{k=1}^N w_k f_{ik} u_{jk} \quad N = 35, w_1 = w_{1,1} w_2 = w_{1,2} \dots w_7 = w_{1,7},$$

$$\begin{aligned} w_8 &= w_{2,1} & \dots & w_{15} = w_{2,7} \\ &\vdots & & \\ &\vdots & & \\ &\vdots & & \\ w_{35} &= w_{5,7} \end{aligned}$$

where the weights w_k are given by the integration formula. Here the components of the vectors f_i are the values of the corresponding harmonic functions of the basic set 1, $\operatorname{Re} z$, $\operatorname{Im} z$, $\operatorname{Re} z^2 \dots$, in the cases a , b ; or of the set u_0 , $\operatorname{Re} z$, \dots , in case c , at the 35 points given by the integration rule.

The approximate solution $u(x, y)$ of the Dirichlet problem is given then by the sum

$$u(x, y) = \sum_{i=1}^n d_i f_i(x, y)$$

where

$$d_i = \sum_{k=1}^i (U, u_k) a_{ki} \quad i = 1, 2, \dots, n.$$

U is a vector the components of which are given by the boundary values of the Dirichlet problem in the points defined by the integration rule; $f_i(x, y)$ is the harmonic function corresponding to the vector f_i .

$u(x, y)$ has the property that among all the possible approximations of the form

$$\sum_{k=1}^n c_k f_k(x, y)$$

the deviation from the exact solution $U_e(x, y)$ is least in the least square sense:

$$\text{if } \Delta = U_e - \sum_{i=1}^n d_i f_i(x, y) = U_e - u$$

$$\text{then } (\Delta, \Delta) = (U_e - u, U_e - u) = \text{minimum.}$$

Nehari [1] has given the following estimate for the deviation in the region where the Dirichlet problem is defined

$$(U_e(x, y) - \sum_{i=1}^n d_i f_i(x, y))^2 \leq (\Delta, \Delta) \cdot \left| \frac{1}{2\pi^2} \int_c \frac{dS}{(X-x)^2 + (Y-y)^2} - \sum_{i=1}^n u_i^2(x, y) \right|.$$

3. Numerical results. For each of the three cases a , b , and c the number n of harmonic functions in the basic set was varied in cases a and b from 3 to 11, in case c from 4 to 12. Due to the limitations in internal storage capacity it was not possible to go higher than 12. The functions were numbered in the following way

$$f_1 = 1, \quad f_2 = \operatorname{Re} z = x, \quad f_3 = \operatorname{Im} z = y, \quad f_4 = \operatorname{Re} z^2 = x^2 - y^2, \quad f_5 = \operatorname{Im} z^2 = 2xy$$

$$f_6 = \operatorname{Re} z^3, \quad f_7 = \operatorname{Im} z^3, \quad f_8 = \operatorname{Re} z^4, \quad f_9 = \operatorname{Im} z^4, \quad f_{10} = \operatorname{Re} z^5, \quad f_{11} = \operatorname{Im} z^5.$$

The variation of n was done in order to observe the convergence of the approximations to the exact solution of the Dirichlet problem. Due to the limited accuracy of the numerical computations (the orthonormalizing code works with floating decimal numbers containing only 8 digits) it must be expected that the improvement of the approximation with increasing n will level off until the addition of another

harmonic function f_i to the set will not improve the approximation at all. In the three cases this point has not yet been reached, as one can see from table 1, in which the norm of the vector consisting of the deviations in the points given by the integration rule is listed.

TABLE 1. Norm of Error Vector Δ
Harmonic Functions

Case	f_1, f_2, f_3	f_1 to f_5	f_1 to f_7	f_1 to f_9	f_1 to f_{11}
<i>a</i>	18.007	9.565	8.822	2.500	2.061
<i>b</i>	.351	.214	.157	.107	.076
c_1^*	.176	.100	.094	.081	.057
c_2^*	.126	.077	.026	.023	.022
c_3^*	.219	.158	.149	.115	.113
c_4^*		.099	.059	.038	.037
c_5^*				.086	.078

* In these cases u_0 was used in addition to f_1, \dots, f_n , and c_i is the case where the boundary values are one on the side i (see Figure 1) and zero on the rest of the boundary. One observes that in the case *a* the norm decreases more rapidly between $n = 7$ and 9. The norm for $n = 8$ is 2.517 and shows that the decrease occurs if $Re z^4$ is added to the set. The explanation for this behavior is probably that the function $Re z^4 = x^4 + y^4 - 6x^2y^2$ with its changes of sign along the lines $x = (\pm 1 \pm \sqrt{2})y$ (all combinations of signs are possible) fits particularly well the prescribed boundary conditions.

In table 2 the maximum error is given for the points on the boundary defined by the integration rule.

TABLE 2

Maximum Error in the Boundary Points Defined by the Integration Rule

Number of functions	3	5	7	9	11	Max. bdry value
Case						
<i>a</i>	11.832	5.739	4.825	1.480	.988	12.915
<i>b</i>	.232	.148	.109	-.087	-.066	.595
c_1^*	-.146	-.065	-.078	-.068	-.052	1.0
c_2^*	-.106	-.055	-.029	-.031	-.028	1.0
c_3^*	-.154	-.115	-.095	-.091	-.095	1.0
c_4^*		-.077	.032	.033	.034	1.0
c_5^*				.070	.079	1.0

From this table one sees that with eleven vectors the maximum relative error in cases *a* and *b* is approximately 10% on the boundary. (Since the deviation has been evaluated only in a finite number of points it is of course possible that this error may be in some points somewhat larger.) In cases c_i the relative error is in most cases smaller than 10% due to the use of an additional harmonic function u_0 in the basic set. One remarks also that the maximum relative error for the first few approximations to the harmonic measures is much smaller than the error in the

cases a and b . This is due to the use of the corresponding harmonic measure u_0 for the circumscribed circle which gives a fairly good first approximation. From these observations one can conclude that from the numerical point of view the basic set of harmonic functions which has to be orthonormalized should not be chosen arbitrarily. The present computations show that a sophisticated choice of these functions creates considerably better approximations for the same number of orthonormal functions.

The Nehari estimates for the deviations in the point $x = y = 0$ are given for the cases a and b in table 3.

TABLE 3. *Deviations at $x = y = 0$ and Nehari Estimates.*

<i>Harmonic functions</i>	f_1 to f_3	f_1 to f_6	f_1 to f_7	f_1 to f_9	f_1 to f_{11}
<i>Case</i>					
a Nehari estimate	5.19	2.74	2.41	.643	.528
actual error (abs.)	.855	.495	.646	.0163	.0133
b Nehari estimate	.1010	.0612	.0428	.0276	.0195
actual error (abs.)	.0099	.0015	.0050	.0017	.0002

From this table one sees that the estimate is still considerably larger than the actual error and that it converges slower than the actual error with increasing number of harmonic functions. If one compares, however, this estimate to the maximum error on the boundary given by table 2 it is evident that the Nehari estimate gives better error bounds than the one which can be derived from the maximum modulus principle for harmonic functions. In table 4 the Nehari estimates for the cases a and b are given for a number of points in the interior of the pentagon and for 11 harmonic polynomials.

TABLE 4

<i>Case</i>	$(y = 0)$	$x = -2$	$x = -1$	$x = 0$	$x = 1$	$x = 2$	$x = 3$
a Nehari estimate	1.798	.539	.528	.528	.614	1.631	
actual error	.052	.094	.0133	.0105	.0181	.406	
b Nehari estimate	.0663	.0199	.0195	.0195	.0226	.0601	
actual error	.0091	.0023	.0002	.0021	.0038	.0086	

Table 4 shows that the Nehari estimates become worse as the boundary of the region is approached if they are compared with the estimates given by the maximum modulus principle. With respect to the actual error, however, the Nehari estimates are further off near the middle of the region than near the boundary.

In table 5 the Nehari estimates for the harmonic measures of the sides in the case where 12 harmonic functions were used are given for $x = y = 0$ together with the maximum error in the points of the boundary given by the integration rule.

In these cases a comparison to the exact error is no longer possible since the exact solution is not known. The values show however that the Nehari estimate gives a better bound for the error at the origin than the one suggested by the maximum error on the boundary.

TABLE 5

Nehari Estimates at $x = y = 0$ and Maximum Error for Harmonic Measures

Case	C_1	C_2	C_3	C_4	C_5
Nehari estimate at $x = y = 0$.0146	.00556	.0239	.00945	.0201
Maximum error	-.0520	-.0279	-.0945	.0335	.0788

4. Concluding Remarks. The best approximation in each of the seven cases gave values which are exact within at most ten per cent for many points of the region. Similar computations by P. Davis and P. Rabinowitz [6] show that with the given limited accuracy of the code the addition of further harmonic polynomials beyond $\text{Im } z^5$ would probably no longer improve this result considerably due to the influence of the round-off errors. In order to improve the accuracy one probably has to use at least double precision in the computations.

The numerical examples given on the previous pages show that the Nehari estimate gives a considerably better bound for the error in the interior of the region than the maximum modulus principle. With respect to the actual error the Nehari estimate is, however, still off by a factor which varied in the examples from 5 to almost 100. It may be that the situation improves if more harmonic polynomials are used with a double precision code, but this can be decided only by experiments using computing machines which have a larger high speed memory than the SEAC. Since the use of orthonormal functions for solving problems in potential theory seems particularly attractive if the solution has to be known only in certain points of the region it would be interesting to see how much the present results can be improved by using double precision codes on the faster large computers like the IBM 704 or Remington Rand 1103AF.

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