NUMERICAL TECHNIQUE FOR SOLVING LEAST-SQUARES PROBLEMS ARISING IN SCATTERING PROBLEM

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1. INTRODUCTION

We consider a least-squares problem that

PROB.1 Find the A_m-coefficients that make the norm

$$\| \sum_{m=1}^{M} A_m(M)\phi_m - f \| = \left[\int_0^1 \left| \sum_{m=1}^{M} A_m(M)\phi_m(x) - f(x) \right|^2 dx \right]^{1/2} \quad (1)$$

minimum. Here, ϕ_m's are basis functions, and f is a given function.

Such a least-squares problem often arises in numerical approach of scattering problems. There, the interval [0,1] corresponds to the boundary of a scatterer and the functions $f(x)$ and $\phi_m(x)$ are the boundary values of an incident wave and the modal functions, respectively. We assume that ϕ_m's and f are the analytic and periodic functions on the interval.

Theoretically speaking, it is obvious that the coefficients are the solutions of the normal equations[1]. And there is no room for doubt. However, in numerical computations, we must discretize the PROB. 1 so that the computer can handle the problem. Here arise two questions :

Q1. How to discretize the problem

Q2. How to solve the discretized problem.

These questions are very important because the accuracy of the evaluated solutoion and the amount of numerical computations directly depend on them.

In this paper, we give the answer for these questions from numerical considerations using the orthogonal decomposition {QR algorithm and SVD(singular Value Decomposition)}[2], which is an efficient numerical technique for solving least-squares problems. As an example, we deal with the least-squares problem which arises in analysing the plane-wave diffraction from a grating by Yasuura's method [3].

2. NUMERICAL TECHNIQUE

As approximation of the norm defined in Eq. (1), the trapezoidal rule is preferable since the integrand is analytic and periodic (This fact is derived from the Euler Maclaurin formula)[1]. Therefore, we discretize the norm as

$$\| \sum_{m=1}^{M} A_m(M,J)\phi_m - f \|_J = \left[\sum_{j=1}^{J} w^2 \left| \sum_{m=1}^{M} A_m(M,J)\phi_m(x_j) - f(x_j) \right|^2 \right]^{1/2}. \quad (2)$$

Here, J is the number of divisions and the sampling points x_j are chosen as

$$x_j = (j-1)/J \qquad (j=1,2,\ldots J), \tag{3}$$

and $w = (1/J)^{1/2}$. Note that we denote the least-squares solutions as $A_m(M,J)$ because the coefficients depend on J in the numerical approach.

Using the vector-matrix notation, the least-squares problem minimizing the norm Eq. (3) is denoted as follows:

PROB. 2 Find the vecotor $\mathbf{A}= [A_1(M,J),A_1(M,J),\ldots,A_1(M,J)]^T$ that make the euclidean norm $\|\Phi\mathbf{A}-\mathbf{f}\|_J$ minimum.

Here, Φ is the Jacobian matrix defined by

$$\Phi = w \begin{bmatrix} \phi_1(s_1), & \phi_2(s_1), & \ldots & ,\phi_M(s_1) \\ \phi_1(s_2), & \phi_2(s_2), & \ldots & ,\phi_M(s_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(s_J), & \phi_2(s_J), & \ldots & ,\phi_M(s_J) \end{bmatrix} \qquad (J\times M), \tag{4}$$

and $\mathbf{f}$ is a J-dimentional complex vector

$$\mathbf{f} = w\ [f(s_1), f(s_2), \ldots, f(s_J)]^T \qquad (^T : \text{transpose}). \tag{5}$$

We employ the orthogonal decomposition method to the discrete least-squares problem (PROB. 2). The SVD or QR algorithm is based on the orthogonal decomposition of the Jacobian Φ [2]. For details on the algorithm, please refer to the literature on numerical analysis, e.g. Refs.[1]-[2]. It should be noted that the Jacobian Φ (or $\mathbf{f}$) is complex .

Singular-Value Decomposition [2]

In this decomposition, the Jacobian Φ is expressed in the form

$$\Phi = U\,S\,V^* \tag{6}$$

where U : a J×M matrix with orthogonal columns [$U^*U=I_M$]
V : an M×M unitary matrix [$V^*V=VV^*=I_M$]
S : an M×M diagonal matrix [$S=\mathrm{diag}(\sigma_1,\sigma_2,\ldots\sigma_M)$]

The diagonal entries σ_j (j=1,2,..M) of S are called the singular values of matrix Φ. Evaluating the values σ_j of Φ, we can calculate the significant quantities such as rank(Φ) (which is the number of non-zero σ_j) and Cond(Φ) ($=\sigma_{max}/\sigma_{min}$). We use this Singular-Value Analysis to investigate the correctness or reasonableness of the discretization of Eqs. (2) and (3).

The least-square solution is evaluated by the decomposition of Eq.(6) {$\mathbf{A}=VS^+U^*\mathbf{f}$ where $S^+=\mathrm{diag}(\sigma_1^+,\sigma_2^+\ldots\sigma_M^+)$ and $\sigma_j^+ = 1/\sigma_j(\sigma_j>0)$; $0\ (\sigma_j=0)$}. However, if it is clear that the Jacobian is full rank, the evaluation of the least-squares solution $\mathbf{A}$ by means of the SVD is not reasonable from points of view of amounts of numerical computations. In such a case, we employ the QR algorrithm.

QR algorithm [2]

When rank(Φ) is equal to M, Φ is decomposed as follows

$$\Phi = Q\,R\,. \tag{7}$$

where Q : a J×M matrix with orthogonal columns [$Q^*Q=I_M$]
R : an M×M upper triangular matrix [rank(R) = M]

Then, the least-squares solution is determined from the equation $R\mathbf{A} = Q^*\mathbf{f}$. It should be noted that R is the regular and triangular matrix.

3. APPLICATION TO YASUURA'S METHOD

As an example, we consider the least-squares problem which arises in analysing the problem of Fourier grating by Yasuura's method.[3,4]

Figure 1 shows the cross section of a Fourier grating and coordinate system. We find the diffracted field when a plane wave

$$F(P) = \exp(ikx \sin\theta - iky \cos\theta) \tag{8}$$

hits the surface of the grating. The approximate wave function for the diffracted fieldis is set up by putting

$$\Psi_N(P) = \sum_{m=-N}^{N} A_m(M)\ \psi_m(P) \qquad (M = 2N+1) \tag{9}$$

$$\psi_m(P) = \exp\{i(k\sin\theta + 2m\pi/d)x + i\beta_m y\} \tag{10}$$

$$\beta_m = \{k^2 - (k\sin\theta + 2m\pi/d)^2\}^{1/2} \quad \mathrm{Re}\{\beta_m\} \geqq 0; \mathrm{Im}\{\beta_m\} \geqq 0$$

The numerical algorithm of Yasuura's method reduces to the PROB.1[3,4]. Namely, the expansion coefficients $A_m(M)$ are given as the solution of the least-squares problem where $\phi_m(x) = \exp(-ikx\sin\theta)\psi_m[x, \eta(x)]$ and $f(x) = \exp(-ikx\sin\theta)F[x, \eta(x)]$.

First, we show the result of the singular value analysis. Figure 2 shows σ_{max} , σ_{min}, cond(Φ), Ω_M and ε_M as functions of J , where M = 21 (N=10). Here, $\Omega_M = \| \Phi\mathbf{A} - \mathbf{f} \|_J^{\ 2}$ and ε_M is the energy error [3]. In this figure, all the quantities become constant for J not less than 2M (=42), as expected from the results stated in Ref. 3. This tendency is common to any other choice of the parameters M (or N), k, θ etc. From the singular value analysis, it is confirmed that the choice

$$J = 2M \tag{11}$$

is sufficient for approximating the PROB. 1 ,

As σ_{min} is not equale to zero as shown in Fig.2, the Jacobian Φ is full rank. Therefore, it is confirmed that we employ the QR algorithm to evaluate solutions of the discretized least-squares problem. To show the effectiveness of the algorithm, in Fig. 3, we compare the errors Ω_M and ε_M of solutions by the QR algorithm with those of thenormal equation. The numerical trouble in the normal equation as observed in Fig. 3 is a typical example of ill-condition [1,2].

We conclude the numerical approach to the least-squares problem of Yasuura's method : (A1) We choose the number of equi-spaced sampling points to be twice as much as the total number of basis functions (J=2M) ; (A2) We employ the QR algorithm to the discretized least-least squares problem.

ACKNOWLEDGMENTS The authors wish to express their thanks to T.Itakura and H.Ikuno of Kumamoto University for useful discussions and continuous encouragements.

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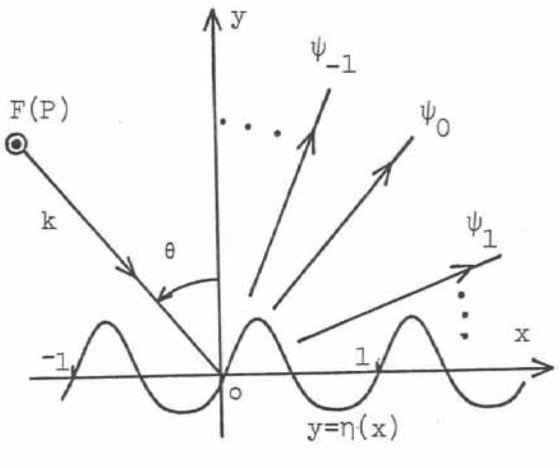

Fig. 1 Cross section of a Fourier grating whose profile is given by $y=\eta(x)=h\{\sin 2\pi x+\gamma\sin(4\pi x+\delta)\}$.

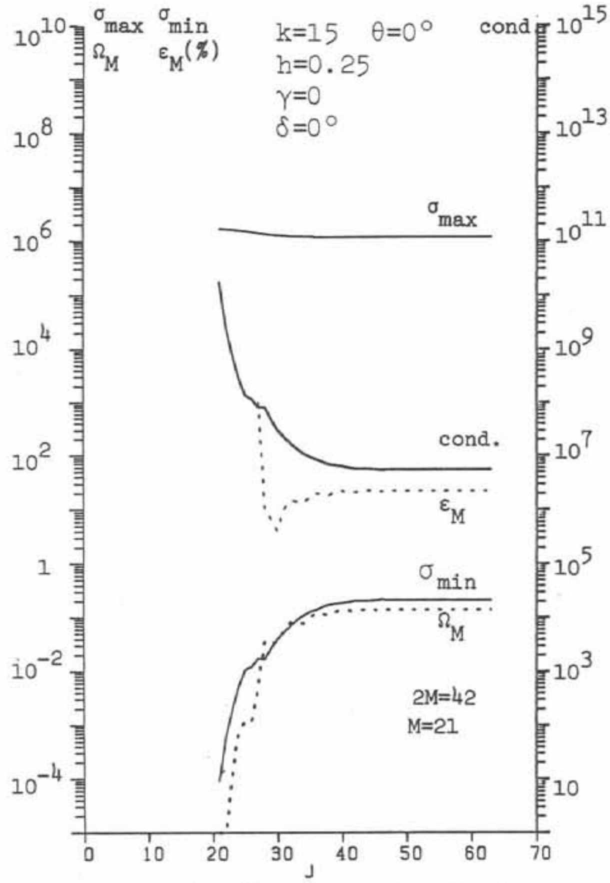

Fig. 2 Singular Value Analysis

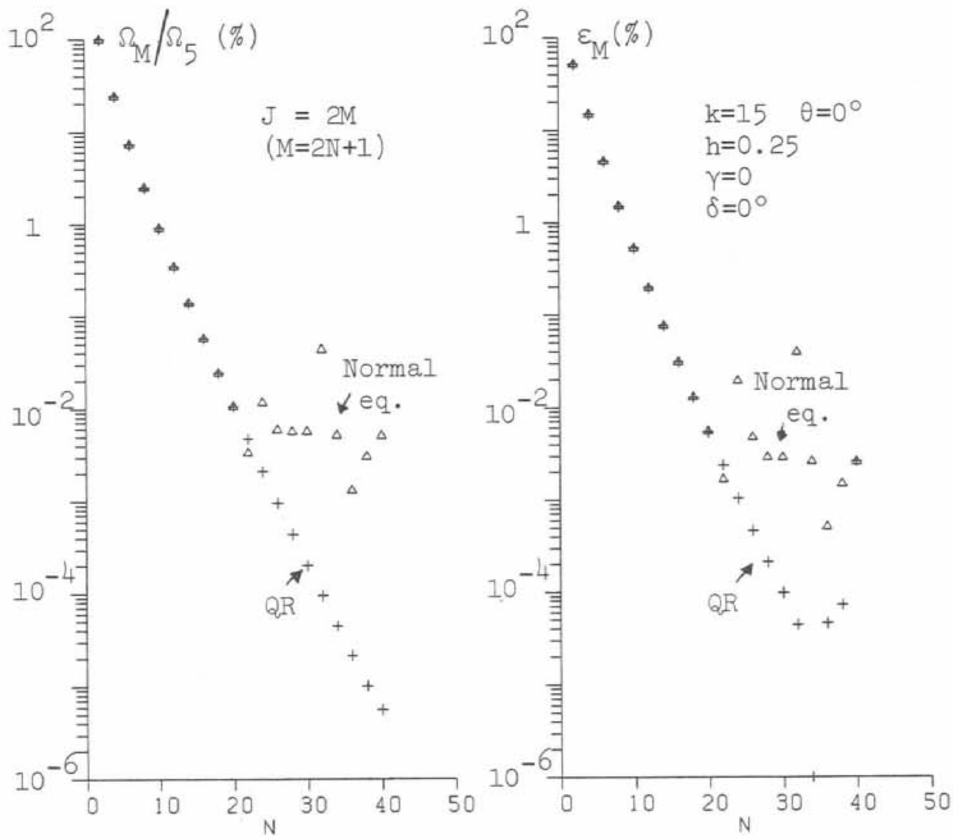

Fig. 3 Comparison of QR algorithm and Normal equation.