Correspondence

On a Sub-Program to determine the Rayleigh Quotient by Conjugate Gradient Method

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Introduction

This paper is represented for a sub-program in order to determine the eigenvalue with respect to the continuous elastic system by applying the conjugate gradient method to Rayleigh quotient. This numerically computational method has been known as iterative method, and frequently used in order to compute the algeraic equation with several variables or large dimensional algebraic equation for elastic-plastic problems by Yamada [1]. The auther also reported for eigenvalue problems of the continuous system in which this method were applied to Rayleigh quotient [2].

The advantages which this method is used are expressed in Ref. [3], therefore they are abbreviated in this paper. In applying this method Rayleigh quotient is used in order to numerically compute the eigenvalue instead of directly computing its from other method. The results are illustrated for the typical engineering examples.

1 Analysis System for Eigenvalue

Consider the continuous elastic system subjected to the concentrated axial forces, as shown in Fig. 1. In which ρ, A, EI and L are density per unit length, cross-sectional area, bending rigidity and total length of beam, respectively.

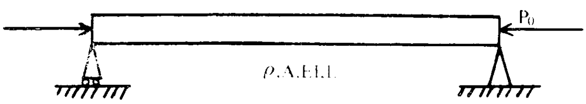

Fig. 1. Simply supported beam subjected to axial forces

The characteristic equations of eigenvalue of dynamic and static problems are generally expressed as,

$$\{[Ke]-P_0[Kg]-\Omega^2[M]\}\vec{q}=0, \tag{1}$$

or

$$\{[Ke]-\lambda[Kg]\}=0. \tag{2}$$

In which $[Ke]$, $[Kg]$ and $[M]$ are total stiffness, stability and mass matrices, respectively, Ω eigen cicular frequency when the beam is subjected to the concentrated axial loads,

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λ critical value of buckling. Note that Eqs. (1) and (2) are formulated by the standard finite element method. The solution of the above equations can be obtained by computing the determinant as follow,

$$|[Ke]-P_0[Kg]-\Omega^2[M]|=0, \tag{3}$$

or

$$|[Ke]-\lambda[Kg]|=0. \tag{4}$$

Note that eigen circular frequency of free vibration can be directly obtained from Eq.(3) in $P_0=0$.

2 Algorithm of Conjugate Gradient Method

In this paper, Rayleigh quotient is used in order to obtained the eigenvalue instead of directly computing of Eqs. (3) and (4) stated above. The algorithm is shown as follow. The Rayleigh quotient for dynamic and static problems is expressed as,

$$R_i=\frac{\vec{q}_i^T[M]\vec{q}_i}{\vec{q}_i^T[K]\vec{q}_i}, \tag{5}$$

in which note that matrix $[Kg]$ in the stability problems is corresponding to matrix $[M]$ in the dynamic problems.

The value of this quotient will be a minimum when the displacement vector $\vec{q}$ is that which most closely approximates the actual mode shape. The applying the conjugate gradient method to Eq. (5), it is, in the first, necessary to find the $\vec{g}_i$ of R_i. Differentiating Eq. (5) with respect to $\vec{q}_i^T$ in order to obtain $\vec{g}_i$ yields subsequently,

$$\frac{\partial R_i}{\partial \vec{q}_i^T}=\frac{2}{\vec{q}_i^T[M]\vec{q}_i}([K]\vec{q}_i-R_i[M]\vec{q}_i),$$

therefore, the direction of gradient is difined by

$$\vec{g}_i=[K]\vec{q}_i-R_i[M]\vec{q}_i. \tag{6}$$

The minimization proceeds step i to step $i+1$ by computing vector $\vec{q}_{i+1}$ in step $i+1$ from vector $\vec{q}_i$ in step i as follow,

$$\vec{q}_{i+1}=\vec{q}_i+\alpha_i\vec{P}_i.$$

where vector $\vec{P}_{i+1}$ is orthogonal with respect to $[K]$, and α_i is determined by minimizing R_i. The substitution of Eq. (7) into Eq. (5) and its differentiation with respect to α_i yields subsequently,

$$\frac{\partial R_i}{\partial \alpha_i}=\frac{1}{\vec{q}_i^T[M]\vec{q}_i}(\vec{P}_i^T[M]\vec{q}_{i+1})(\vec{q}_i^T[M]\vec{q}_{i+1})-(\vec{q}_{i+1}^T[K]\vec{q}_{i+1})(\vec{P}_i^T[M]\vec{q}_{i+1}). \tag{7}$$

The minimum value of R will occur where this partial derivative in zero. The extreme value will be obtained by solving the following equation,

$$(\vec{P}_i^T[K]\vec{q}_{i+1})(\vec{q}_{i+1}^T[M]\vec{q}_{i+1})-(\vec{q}_{i+1}^T[K]\vec{q}_{i+1})(\vec{P}_i^T[M]\vec{q}_{i+1})=0. \tag{8}$$

Substituting Eq. (7) into Eq. (8), the quadratic equation with respect to α_i can be subsequently obtained as,

$$a\alpha_i^2 + b\alpha_i + c = 0,$$

where the coefficients a, b and c are of the forms as,

$$a = (\vec{P}_i^T[K]\vec{P}_i)(\vec{q}_i^T[K]\vec{P}_i) - (\vec{q}_i^T[K]\vec{P}_i)(\vec{P}_i^T[M]\vec{P}_i),$$

$$b = (\vec{P}_i^T[K]\vec{P}_i)(\vec{q}_i^T[M]\vec{q}_i) - (\vec{q}_i^T[K]\vec{q}_i)(\vec{q}_i^T[M]\vec{P}_i),$$

$$c = (\vec{q}_i^T[K]\vec{P}_i)(\vec{q}_i^T[M]\vec{q}_i) - (\vec{q}_i^T[K]\vec{q}_i)(\vec{P}_i^T[M]\vec{q}_i).$$

The two roots with respect to α_i are computed from

$$\alpha_i = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \; ; (i = 1, 2).$$

One of the two roots can be selected to minimizing quotient R obtained by substituting these into Eqs. (5) and (7), as shown in Fig. 2.

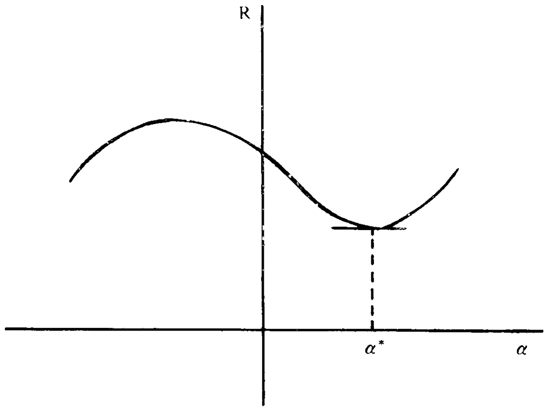

Fig. 2. Representative variation of Rayleigh quotient a line

Vector $\vec{P}_{i+1}$ in step $i+1$ is determined from the gradianet $\vec{g}_{i+1}$ and vector $\vec{P}_i$ obtained from the previous step by using the following formula,

$$\vec{P}_{i+1} = \vec{g}_{i+1} + \beta_i \vec{P}_i \tag{9}$$

where β_i is a constant coefficient and is found by requiring that $\vec{P}_i$ and $\vec{P}_{i+1}$ are orthogonal with respect to $[K]$. Therefore the value of β_i is given by,

$$\beta_i = -\frac{\vec{P}_i^T[K]\vec{q}_{i+1}}{\vec{P}_i^T[K]\vec{P}_i} \tag{10}$$

The algorithm can be surmarized as,

1. Initialization ($i=0$)

$$\vec{q}_0 = \text{given arbitrary constant},$$

$\vec{g}_0 = R(\vec{q}_0)$,

$\vec{P}_0 = \vec{g}_0$.

2. Next step iteration

(1) compute α_i,

(2) compute $\vec{q}_{i+1} = \vec{q}_i + \alpha_i \vec{P}_i$,

(3) compute $R_{i+1} = \dfrac{\vec{q}^T_{i+1}[K]\vec{q}_{i+1}}{\vec{q}^T_{i+1}[M]\vec{q}_{i+1}}$

(4) compute $\vec{g}_{i+1} = [K]\vec{q}_{i+1} - R_{i+1}[M]\vec{q}_{i+1}$

(5) compute $\beta = -\dfrac{\vec{P}^T_i[K]\vec{g}_{i+1}}{\vec{P}^T_i[K]\vec{P}_i}$

(6) compute $\vec{P}_{i+1} = \vec{g}_{i+1} + \beta_i \vec{P}_i$

The iteration are carried out to obtained the convergent value of R. The then convergent value can be given as follow,

$$|R_{i+1} - R_i| < e,$$

where e is the condition of covergence.

3 Numerical Example and Conlusion

Consider the simply supported uniform beam subjected to the concentrated axial forces at both ends, as shown in Fig. 1. In which mass, stiffness and stability matrices can be obtained by means of applying the standard finite element method, respectively. These are denoted as follow,

$$[m] = \frac{\rho A l}{420}\begin{bmatrix} 156 & 22l & 54 & -13l \\ 22l & 4l^2 & 13l & -3l^2 \\ 54 & 13l & 156 & -22l \\ -13l & -3l^2 & -22l & 4l^2 \end{bmatrix},$$

$$[k_e] = \frac{EI}{l^3}\begin{bmatrix} 12 & 6l & -12 & 6l \\ 6l & 4l^2 & -6l & 2l^2 \\ -12 & -6l & 12 & -6l \\ 6l & 2l^2 & -6l & 4l^2 \end{bmatrix},$$

$$[k_g] = \frac{P_0}{l}\begin{bmatrix} 6/5 & l/10 & -6/5 & l/10 \\ l/10 & 2l^2/15 & -l/10 & -l^2/30 \\ -6/5 & -l/10 & 6/5 & -l/10 \\ l/10 & -l^2/30 & -l/10 & 2l^2/15 \end{bmatrix}.$$

Each of the above element matrices must be assembled for the given entire structural system when these are employed to practical problems. R value corresponding to eigenvalue, ω^2, of transverse free vibration and critical buckling value, P_{cr}, can be expressed as follow,

$$R=\omega^2\frac{\rho AL^4}{EI}=\frac{\vec{q}_i^T[Ke]\vec{q}_i}{\vec{q}_i^T[M]\vec{q}_i}=\pi^4,$$

$$R=P_{cr}\frac{L^2}{EI}=\frac{\vec{q}_i^T[Ke]\vec{q}}{\vec{q}_i^T[Kg]\vec{q}_i}=\pi^2.$$

The results are shown for two kinds of the finite element in Table 1. The each of (2) and (4) in Table 1 expressed on the divided number of finite elements. The results are expressed that the four divided finite elements are sufficiently satistied when the computation is carried out for the practical problems.

Table 1 A Comparison of eigenvalues

	$\sqrt{\omega^2\frac{\rho AL^4}{EI}}$	error %	$P_{cr}\frac{L^2}{EI}$	error %
Theory	9.87		9.87	
Present solution	9.91(2)	0.4	9.94(2)	0.7
	9.88(4)	0.1	9.89(4)	0.2

The sub-program is shown in Appendix. Note that $EPS=10^{-5}$ for the condition of convergence and total length $L=450$ [mm] of the beam are given in order to carry out this computation.

4 Acknowledgement

The FACOM 230–38 in Kokushikan University Computer Center has been used for the objective computation.

(Recieved 18 January 1982)

References

1) Yamada, *et al.*, EPIC-IV, (in Japanese), (1980), BAIFUKAN.
2) K. Shimoyamada, *Prescript* JSME, (in Japanese), No. 760-1, (June, 1976), p 69.
3) K. Shimoyamada, Memoris of the Kokushikan University Computer Center, No.2, (march, 1981), p 15.
4) Rubinstein, M.F., *et al.*, J. Franklin Inst. Vol. 293, No. 3, (march, 1972), p173.

Appendix

This appendix shows the program for algorithm represented in this paper. When this program is used, we would be required to prepare the subroutine in order to operate, for example, the form of "$\vec{q}^T[K]\vec{q}$" and to clear the vector (VECMAT and CLVEC in this program, respectively)

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FACOM 230 CS2/VS     FORTRAN S                      V-03 L-70       DATE 62.01.28  TIME 14.26  PAGE 0001

SOURCE    LIST

            C      *** CONJUGATE GRADIENT METHOD *******
            C      AK-CORRESPONDING TO STIFFNESS MATRIX
            C      BM-CORRESPONDING TO MASS OR STABILITY MATRIX
            C      Q-DISPLACEMENT VECTOR
            C      D-JUDGEMENT OF ROOT OF QUADRATIC EQUATION
            C      NRED- DIMENSION FOR CALCURATION
            C      NELM-DIMENSION OF MATRIX
0001               SUBROUTINE FUMCG(AK,BM,RAL,D,NRED,NELM,Q,EPS)
            C **
0002               DIMENSION AK(NELM,NELM),BM(NELM,NELM),Q(NELM)
0003               DIMENSION P(30),QQ(30),QD(30),OLDP(30),OLDQ(30),C(30),GG(30)
            C **
            C      COMPUTE FOR INITIAL ARGUMENT*
0004               CALL CLVEC(Q,NELM)
            C      ARBITRARY VALUE GIVEN TO ALL COMPONENT OF DISPLACEMENT Q(I)
0005               DO 20 I=1,NRED
0006            20 Q(I)=1.0
            C      COMPUTE THE EACH FACTOR FOR INITIAL RAYLEIGH QUOTIENT
0007               CALL CLVEC(C,NELM)
0008               CALL VECMAT(C1,Q,Q,AK,C,NRED,NELM)
0009               CALL CLVEC(C,NELM)
0010               CALL VECMAT(C2,Q,Q,BM,C,NRED,NELM)
            C      COMPUTE THE INITIAL RAYLEIGH QUOTIENT
0011               RAL=C1/C2
0012               WRITE(6,50) RAL
            C      COMPUTE THE GRADIENT VECTOR GG(I)
0013               DO 60 I=1,NRED
0014               S=0.0
0015               DO 70 J=1,NRED
0016               S=S+(AK(I,J)-RAL*BM(I,J))*Q(J)
0017            70 CONTINUE
0018               GG(I)=S
0019            60 CONTINUE
            C      **** ORTHOGONAL VECTOR ***** P(I)     ****
0020               DO 80 I=1,NRED
0021               P(I)=GG(I)
0022            80 CONTINUE
            C      *** NEXT STEP ITERATION *****
0023               K=0
0024          1000 CONTINUE
0025               K=K+1
0026               R=RAL
0027               DO 90 I=1,NRED
0028               OLDQ(I)=Q(I)
0029               OLDP(I)=P(I)
0030            90 CONTINUE
0031               CALL CLVEC(P,NELM)
0032               CALL CLVEC(Q,NELM)
0033               CALL CLVEC(GG,NELM)
            C      COMPUTE THE FACTOR OF QUADRATIC EQUATION
0034               CALL VECMAT(D1,OLDP,OLDP,AK,C,NRED,NELM)
0035               CALL CLVEC(C,NELM)
0036               CALL VECMAT(D2,OLDQ,OLDP,BM,C,NRED,NELM)
0037               CALL CLVEC(C,NELM)
0038               CALL VECMAT(D3,OLDQ,OLDP,AK,C,NRED,NELM)
0039               CALL CLVEC(C,NELM)
0040               CALL VECMAT(D4,OLDP,OLDP,BM,C,NRED,NELM)
0041               AA=(D1*D2)-(D3*D4)
0042               CALL CLVEC(C,NELM)
0043               CALL VECMAT(D1,OLDP,OLDP,AK,C,NRED,NELM)
0044               CALL CLVEC(C,NELM)
0045               CALL VECMAT(D2,OLDQ,OLDQ,BM,C,NRED,NELM)
0046               CALL CLVEC(C,NELM)
0047               CALL VECMAT(D3,OLDQ,OLDQ,AK,C,NRED,NELM)
0048               CALL CLVEC(C,NELM)
0049               CALL VECMAT(D4,OLDP,OLDP,BM,C,NRED,NELM)
0050               CALL CLVEC(C,NELM)
0051               BB=(D1*D2)-(D3*D4)
0052               CALL VECMAT(D1,OLDP,OLDQ,AK,C,NRED,NELM)
0053               CALL CLVEC(C,NELM)
0054               CALL VECMAT(D2,OLDQ,OLDQ,BM,C,NRED,NELM)
0055               CALL CLVEC(C,NELM)
0056               CALL VECMAT(D3,OLDQ,OLDQ,AK,C,NRED,NELM)
0057               CALL CLVEC(C,NELM)
0058               CALL VECMAT(D4,OLDP,OLDQ,BM,C,NRED,NELM)
0059               CC=(D1*D2)-(D3*D4)
0060               CALL QUAD(AA,BB,CC,D,X1,X2)
0061               IF(D.LT.0.0) GO TO 1520
            C      *** COMPUTE THE DISPLACEMENT VECTOR QQ QD,******
0062               DO 100 I=1,NRED
0063               QQ(I)=OLDQ(I)+X1*OLDP(I)
0064               QD(I)=OLDQ(I)+X2*OLDP(I)
0065           100 CONTINUE
            C      *** COMPUTE THE  RAYLEIGH QUOTIENT RAL IN N-STEP
0066               RAL=0.0
0067               CALL CLVEC(C,NELM)
0068               CALL VECMAT(D1,QQ,QQ,AK,C,NRED,NELM)
0069               CALL CLVEC(C,NELM)
0070               CALL VECMAT(D2,QQ,QQ,BM,C,NRED,NELM)
0071               CALL CLVEC(C,NELM)
0072               CALL VECMAT(D3,QD,QD,AK,C,NRED,NELM)
0073               CALL CLVEC(C,NELM)
0074               CALL VECMAT(D4,QD,QD,BM,C,NRED,NELM)
0075               RAL1=D1/D2
0076               RAL2=D3/D4
0077               IF(RAL1.LT.RAL2.AND.RAL1.GT.0.0) GO TO 2000
0078               RAL=RAL2
0079               IF(RAL.LT.0.0) GO TO 1500
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SOURCE    LIST

          DO 110 I=1,NRED
          Q(I)=QD(I)
    110   CONTINUE
          IF(ABS(R-RAL).LT.EPS) GO TO 1510
          GO TO 1600
   2000   CONTINUE
          RAL=RAL1
          IF(RAL.LT.0.0) GO TO 1500
          DO 120 I=1,NRED
    120   Q(I)=QQ(I)
          IF(ABS(R-RAL).LT.EPS) GO TO 1510
  C       **** COMPUTE THE N-STEP GRADIENT VECTOR ******
   1600   CONTINUE
          DO 130 I=1,NRED
          S=0.0
          DO 140 J=1,NRED
          S=S+(AK(I,J)-RAL*BM(I,J))*Q(J)
    140   CONTINUE
          GG(I)=S
    130   CONTINUE
  C       *** COMPUTE THE ORTHOGONAL  VECTOR P  TO AK
          CALL CLVEC(C,NELM)
          CALL VECMAT(D1,OLDP,GG,AK,C,NRED,NELM)
          CALL CLVEC(C,NELM)
          CALL VECMAT(D2,OLDP,OLDP,AK,C,NRED,NELM)
          BETA=-(D1/D2)
          DO 160 I=1,NRED
          P(I)=(GG(I)+BETA*OLDP(I))
    160   CONTINUE
          CALL CLVEC(C,NELM)
          CALL CLVEC(OLDP,NELM)
          CALL CLVEC(OLDQ,NELM)
          GO TO 1000
   1510   WRITE(6,200) K
          WRITE(6,180) RAL1,RAL2,RAL
          RETURN
   1500   WRITE(6,170)
          RETURN
   1520   WRITE(6,190)
          RETURN
     50   FORMAT(/5X,4HRAL=,E15.7)
    170   FORMAT(/5X,30X,'0H** OBTAINED NEGATIVE RALEIGH QUONTIENT** ')
    180   FORMAT(1H ,5X,5HRAL1=,E15.7,10X,5HRAL2=,E15.7,10X,4HRAL=,E15.7)
    190   FORMAT(/5X,' *OBTAINED NEGATIVE ROOT OF QUADRATIC EQUATION * ')
    200   FORMAT(1H ,I5,1X,14HSTEP ITERATION)
          END
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