Matrix Iteration

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Outline

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Introduction

Dynamic analysis of MDOF systems based on modal superposition is both simple and efficient

- simple: the modal response can be easily computed, analitically or numerically, with the techniques we have seen for SDOF systems,
- efficient: in most cases, only the modal responses of a few lower modes are required to accurately describe the structural response.

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Introduction

As the structural matrices are easily assembled using the *FEM*, our modal superposition procedure is ready to be applied to structures with tenth, thousands or millions of *DOF*'s! except that we can compute the eigenpairs only when the analyzed structure has two, three or maybe four degrees of freedom...
We will discuss how it is possible to compute the eigenpairs of arbitrary dynamic systems using the so called *Matrix Iterations* procedure and a number of variations derived from this fundamental idea.

Equilibrium

First, we will see an iterative procedure whose outputs are the first, or fundamental, mode shape vector and the corresponding eigenvalue.
When an undamped system freely vibrates with a harmonic time dependency of frequency ω_i, the equation of motion, simplifying the time dependency, is

$$\mathbf{K}\,\boldsymbol{\psi}_i = \omega_i^2 \mathbf{M}\,\boldsymbol{\psi}_i.$$

In equilibrium terms, the elastic forces are equal to the inertial forces when the systems oscillates with frequency ω_i^2 and mode shape $\boldsymbol{\psi}_i$

Proposal of an iterative procedure

Our iterative procedure will be based on finding a new displacement vector $\mathbf{x}_{n+1}$ such that the elastic forces $\mathbf{f}_S = \mathbf{K}\,\mathbf{x}_{i+1}$ are in equilibrium with the inertial forces due to the *old* displacement vector $\mathbf{x}_n$, $\mathbf{f}_I = \omega_i^2 \mathbf{M}\,\mathbf{x}_n$, that is

$$\mathbf{K}\,\mathbf{x}_{n+1} = \omega_i^2 \mathbf{M}\,\mathbf{x}_n.$$

Premultiplying by the inverse of $\mathbf{K}$ and introducing the *Dynamic Matrix*, $\mathbf{D} = \mathbf{K}^{-1}\mathbf{M}$

$$\mathbf{x}_{n+1} = \omega_i^2 \mathbf{K}^{-1}\mathbf{M}\,\mathbf{x}_n = \omega_i^2 \mathbf{D}\,\mathbf{x}_n.$$

In the generative equation above we miss a fundamental part, the square of the free vibration frequency ω_i^2.

The Matrix Iteration Procedure, 1

This problem is solved considering the $\mathbf{x}_n$ as a sequence of *normalized* vectors and introducing the idea of an *unnormalized* new displacement vector, $\hat{\mathbf{x}}_{n+1}$,

$$\hat{\mathbf{x}}_{n+1} = \mathbf{D}\,\mathbf{x}_n,$$

note that we removed the explicit dependency on ω_i^2.

The Matrix Iteration Procedure, 1

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The normalized vector is obtained applying to $\hat{\mathbf{x}}_{n+1}$ a normalizing factor, $\mathfrak{F}_{n+1}$,

$$\mathbf{x}_{n+1} = \frac{\hat{\mathbf{x}}_{n+1}}{\mathfrak{F}_{n+1}},$$

$$\text{but} \qquad \mathbf{x}_{n+1} = \omega_i^2 \mathbf{D}\,\mathbf{x}_n = \omega_i^2\,\hat{\mathbf{x}}_{n+1}, \quad \Rightarrow \quad \frac{1}{\mathfrak{F}} = \omega_i^2$$

If we agree that, near convergence, $\mathbf{x}_{n+1} \approx \mathbf{x}_n$, substituting in the previous equation we have

$$\mathbf{x}_{n+1} \approx \mathbf{x}_n = \omega_i^2\,\hat{\mathbf{x}}_{n+1} \quad \Rightarrow \quad \omega_i^2 \approx \frac{\mathbf{x}_n}{\hat{\mathbf{x}}_{n+1}}.$$

Of course the division of two vectors is not an option, so we want to twist it into something useful.

Normalization

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First, consider $\mathbf{x}_n = \boldsymbol{\psi}_i$: in this case, for $j = 1, \ldots, N$ it is

$$x_{n,j}/\hat{x}_{n+1,j} = \omega_i^2.$$

When $\mathbf{x}_n \neq \boldsymbol{\psi}_i$ it is possible to demonstrate that we can bound the eigenvalue

$$\min_{j=1,\ldots,N}\left\{\frac{x_{n,j}}{\hat{x}_{n+1,j}}\right\} \leqslant \omega_i^2 \leqslant \max_{j=1,\ldots,N}\left\{\frac{x_{n,j}}{\hat{x}_{n+1,j}}\right\}.$$

A more rational approach would make reference to a proper vector norm, so using our preferred vector norm we can write

$$\omega_i^2 \approx \frac{\hat{\mathbf{x}}_{n+1}^T \mathbf{M}\,\mathbf{x}_n}{\hat{\mathbf{x}}_{n+1}^T \mathbf{M}\,\hat{\mathbf{x}}_{n+1}},$$

(if memory helps, this is equivalent to the R_{11} approximation, that we introduced studying Rayleigh quotient refinements).

Proof of Convergence, 1

Until now we postulated that the sequence x_n converges to some, unspecified eigenvector ψ_i, now we will demonstrate that the sequence converge to the first, or fundamental mode shape,

$$\lim_{n\to\infty} x_n = \psi_1.$$

1. Expand x_0 in terms of eigenvectors an modal coordinates:

$$x_0 = \psi_1 q_{1,0} + \psi_2 q_{2,0} + \psi_3 q_{3,0} + \cdots .$$

2. The inertial forces, assuming that the system is vibrating according to the fundamental frequency, are

$$\begin{aligned} f_{I,n=0} &= \omega_1^2 M \left(\psi_1 q_{1,0} + \psi_2 q_{2,0} + \psi_3 q_{3,0} + \cdots\right) \\ &= M\left(\omega_1^2 \psi_1 q_{1,0} \frac{\omega_1^2}{\omega_1^2} + \omega_2^2 \psi_2 q_{2,0} \frac{\omega_1^2}{\omega_2^2} + \cdots\right). \end{aligned}$$

Proof of Convergence, 2

3. The deflections due to these forces (no hat!, we have multiplied by ω_1^2) are

$$x_{n=1} = K^{-1} M \left(\omega_1^2 \psi_1 q_{1,0} \frac{\omega_1^2}{\omega_1^2} + \omega_2^2 \psi_2 q_{2,0} \frac{\omega_1^2}{\omega_2^2} + \cdots\right),$$

(note that every term has been multiplied and divided by the corresponding eigenvalue ω_i^2).

4. With $\omega_j^2 M\, \psi_j = K \psi_j$, substituting and simplifying $K^{-1}K = I$,

$$\begin{aligned} x_{n=1} &= K^{-1}\left(K\psi_1 q_{1,0}\left(\frac{\omega_1^2}{\omega_1^2}\right)^1 + K\psi_2 q_{2,0}\left(\frac{\omega_1^2}{\omega_2^2}\right)^1 + K\psi_3 q_{3,0}\left(\frac{\omega_1^2}{\omega_3^2}\right)^1 + \cdots\right) \\ &= \psi_1 q_{1,0}\frac{\omega_1^2}{\omega_1^2} + \psi_2 q_{2,0}\frac{\omega_1^2}{\omega_2^2} + \psi_3 q_{3,0}\frac{\omega_1^2}{\omega_3^2} + \cdots, \end{aligned}$$

Proof of Convergence, 3

5. applying again this procedure

$$x_{n=2} = \left(\psi_1 q_{1,0}\left(\frac{\omega_1^2}{\omega_1^2}\right)^2 + \psi_2 q_{2,0}\left(\frac{\omega_1^2}{\omega_2^2}\right)^2 + \psi_3 q_{3,0}\left(\frac{\omega_1^2}{\omega_3^2}\right)^2 + \cdots\right),$$

6. applying the procedure n times

$$x_n = \left(\psi_1 q_{1,0}\left(\frac{\omega_1^2}{\omega_1^2}\right)^n + \psi_2 q_{2,0}\left(\frac{\omega_1^2}{\omega_2^2}\right)^n + \psi_3 q_{3,0}\left(\frac{\omega_1^2}{\omega_3^2}\right)^n + \cdots\right).$$

Proof of Convergence, 4

Going to the limit,

$$\lim_{n\to\infty} x_n = \psi_1 q_{1,0}$$

because

$$\lim_{n\to\infty} \left(\frac{\omega_1^2}{\omega_j^2}\right)^n = \delta_{1j}$$

Consequently,

$$\lim_{n\to\infty} \frac{|x_n|}{|\hat{x}_n|} = \omega_1^2$$

Purified Vectors

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If we know ψ_1 and ω_1^2 from the matrix iteration procedure it is possible to compute the second eigenpair, following a slightly different procedure.
Express the initial iterate in terms of the (unknown) eigenvectors,

$$x_{n=0} = \Psi\, q_{n=0}$$

and premultiply by the (known) $\psi_1^T M$:

$$\psi_1^T M\, x_{n=0} = M_1 q_{1,n=0}$$

solving for $q_{1,n=0}$

$$q_{1,n=0} = \frac{\psi_1^T M\, x_{n=0}}{M_1}.$$

Knowing the amplitude of the 1st modal contribution to $x_{n=0}$ we can write a *purified* vector,

$$y_{n=0} = x_{n=0} - \psi_1 q_{1,n=0}.$$

Convergence (?)

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It is easy to demonstrate that using $y_{n=0}$ as our starting vector

$$\lim_{n\to\infty} y_n = \psi_2 q_{2,n=0}, \qquad \lim_{n\to\infty} \frac{|y_n|}{|\hat{y}_n|} = \omega_2^2.$$

because the initial amplitude of the first mode is null.

Due to numerical errors in the determination of fundamental mode and in the procedure itself, using a plain matrix iteration the procedure however converges to the 1st eigenvector, so to preserve convergence to the 2nd mode it is necessary that the iterated vector y_n is purified at each step n.

Purification Procedure

The purification procedure is simple, at each step the amplitude of the 1st mode is first computed, then removed from the iterated vector $\mathbf{y}_n$

$$q_{1,n} = \psi_1^T \mathbf{M} \mathbf{y}_n / M_1,$$

$$\hat{\mathbf{y}}_{n+1} = \mathbf{D} \left(\mathbf{y}_n - \psi_1 q_{1,n} \right) = \mathbf{D} \left(\mathbf{I} - \frac{1}{M_1} \psi_1 \psi_1^T \mathbf{M} \right) \mathbf{y}_n$$

Introducing the *sweeping matrix* $\mathbf{S}_1 = \mathbf{I} - \frac{1}{M_1} \psi_1 \psi_1^T \mathbf{M}$ and the modified dynamic matrix $\mathbf{D}_2 = \mathbf{D}\mathbf{S}_1$, we can write

$$\hat{\mathbf{y}}_{n+1} = \mathbf{D}\mathbf{S}_1 \mathbf{y}_n = \mathbf{D}_2 \mathbf{y}_n.$$

This is known as *matrix iteration with sweeps*.

Third Mode

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Using again the idea of purifying the iterated vector, starting with the knowledge of the first and the second eigenpair,

$$\hat{\mathbf{y}}_{n+1} = \mathbf{D} \left(\mathbf{y}_n - \psi_1 q_{1,n} - \psi_2 q_{2,n} \right)$$

with $q_{n,1}$ as before and

$$q_{2,n} = \psi_2^T \mathbf{M} \mathbf{y}_n / M_2,$$

substituting in the expression for the purified vector

$$\hat{\mathbf{y}}_{n+1} = \mathbf{D} \big(\underbrace{\mathbf{I} - \frac{1}{M_1} \psi_1 \psi_1^T \mathbf{M}}_{\mathbf{S}_1} - \frac{1}{M_2} \psi_2 \psi_2^T \mathbf{M} \big)$$

The conclusion is that the sweeping matrix and the modified dynamic matrix to be used to compute the 3rd eigenvector are

$$\mathbf{S}_2 = \mathbf{S}_1 - \frac{1}{M_2} \psi_2 \psi_2^T \mathbf{M}, \qquad \mathbf{D}_3 = \mathbf{D}\,\mathbf{S}_2.$$

Generalization to Higher Modes

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The results obtained for the third mode are easily generalised.
It is easy to verify that the following procedure can be used to compute all the modes.

Define $\mathbf{S}_0 = \mathbf{I}$, take $i = 1$,

1. compute the modified dynamic matrix to be used for mode i,

$$\mathbf{D}_i = \mathbf{D}\,\mathbf{S}_{i-i}$$

2. compute ψ_i using the modified dynamic matrix;
3. compute the modal mass $M_i = \psi^T \mathbf{M}\, \psi$;
4. compute the sweeping matrix $\mathbf{S}_i$ that *sweeps* the contributions of the first i modes from trial vectors,

$$\mathbf{S}_i = \mathbf{S}_{i-1} - \frac{1}{M_i} \psi_i \psi_i^T \mathbf{M};$$

5. increment i, `GOTO 1`.

Well, we finally have a method that can be used to compute all the eigenpairs of our dynamic problems, full circle!

Discussion

The method of matrix iteration with sweeping is not used in production because

1. $\mathbf{D}$ is a full matrix, even if $\mathbf{M}$ and $\mathbf{K}$ are banded matrices, and the matrix product that is the essential step in every iteration is computationally onerous,
2. the procedure is however affected by numerical errors,

so, after having demonstrated that it is possible to compute all the eigenvectors of a large problem using an iterative procedure it is time to look for different, more efficient iterative procedures.

Introduction to Inverse Iteration

Inverse iteration is based on the fact that the symmetric stiffness matrix has a banded structure, that is a relatively large triangular portion of the matrix is composed by zeroes.

The banded structure is due to the FEM model: in every equation of equilibrium the only non zero elastic force coefficients are due to the degrees of freedom of the few FE's that contain the degree of freedom for which the equilibrium is written.

Definition of LU decomposition

Every symmetric, banded matrix can be subjected to a so called *LU* decomposition, that is, for $\mathbf{K}$ we write

$$\mathbf{K} = \mathbf{L}\,\mathbf{U}$$

where $\mathbf{L}$ and $\mathbf{U}$ are, respectively, a lower- and an upper-banded matrix.
If we denote with b the bandwidth of $\mathbf{K}$, we have

$$\mathbf{L} = \left[l_{ij}\right] \quad \text{with } l_{ij} \equiv 0 \text{ for } \begin{cases} i < j \\ j < i - b \end{cases}$$

and

$$\mathbf{U} = \left[u_{ij}\right] \quad \text{with } u_{ij} \equiv 0 \text{ for } \begin{cases} i > j \\ j > i + b \end{cases}$$

Twice the equations?

In this case, with $\boldsymbol{w}_n = \boldsymbol{M}\,\boldsymbol{x}_n$, the recursion can be written

$$\boldsymbol{L}\,\boldsymbol{U}\,\boldsymbol{x}_{n+1} = \boldsymbol{w}_n$$

or as a system of equations,

$$\begin{aligned}\boldsymbol{U}\,\boldsymbol{x}_{n+1} &= \boldsymbol{z}_{n+1}\\ \boldsymbol{L}\,\boldsymbol{z}_{n+1} &= \boldsymbol{w}_n\end{aligned}$$

Apparently, we have doubled the number of unknowns, but the z_j's can be easily computed by the procedure of *back substitution*.

Back Substitution

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Temporarily dropping the n and $n+1$ subscripts, we can write

$$\begin{aligned}z_1 &= (w_1)/l_{11}\\ z_2 &= (w_2 - l_{21}z_1)/l_{22}\\ z_3 &= (w_3 - l_{31}z_1 - l_{32}z_2)/l_{33}\\ &\dots\\ z_j &= (w_j - \sum_{k=1}^{j-1} l_{jk}z_k)/l_{jj}\\ &\dots\end{aligned}$$

The $\boldsymbol{x}$ are then given by $\boldsymbol{U}\,\boldsymbol{x} = \boldsymbol{z}$.

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We have computed $\boldsymbol{z}$ by back substitution, we must solve $\boldsymbol{U}\,\boldsymbol{x} = \boldsymbol{z}$ but U is upper triangular, so we have

$$\begin{aligned}x_N &= (z_N)/u_{NN}\\ x_{N-1} &= (z_{N-1} - u_{N-1,N}z_N)/u_{N-1,N-1}\\ x_{N-2} &= (z_{N-2} - u_{N-2,N}z_N - u_{N-2,N-1}z_{N-1})/u_{N-2,N-2}\\ &\dots\\ x_{N-j} &= (z_{N-j} - \sum_{k=0}^{j-1} u_{N-j,N-k}z_{N-k})/u_{N-j,N-j},\end{aligned}$$

For moderately large systems, the reduction in operations count given by back substitution with respect to matrix multiplication is so large that the additional cost of the *LU* decomposition is negligible.

Introduction to Shifts

Inverse iteration can be applied to each step of matrix iteration with sweeps, or to each step of a different procedure intended to compute all the eigenpairs, the *matrix iteration with shifts*.

Matrix Iteration with Shifts, 1

If we write

$$\omega_i^2 = \mu + \lambda_i,$$

where μ is a *shift* and λ_i is a *shifted eigenvalue*, the eigenvalue problem can be formulated as

$$\mathbf{K}\,\boldsymbol{\psi}_i = (\mu + \lambda_i)\mathbf{M}\,\boldsymbol{\psi}_i$$

or

$$(\mathbf{K} - \mu\mathbf{M})\boldsymbol{\psi}_i = \lambda_i \mathbf{M}\,\boldsymbol{\psi}_i.$$

If we introduce a modified stiffness matrix

$$\overline{\mathbf{K}} = \mathbf{K} - \mu\mathbf{M},$$

we recognize that we have a *new* problem, that has *exactly* the same eigenvectors and *shifted* eigenvalues,

$$\overline{\mathbf{K}}\,\boldsymbol{\phi}_i = \lambda_i \mathbf{M}\boldsymbol{\phi}_i,$$

where

$$\boldsymbol{\phi}_i = \boldsymbol{\psi}_i, \qquad \lambda_i = \omega_i^2 - \mu.$$

Matrix Iteration with Shifts, 2

The shifted eigenproblem can be solved, e.g., by matrix iteration and the procedure will converge to the *smallest absolute value* shifted eigenvalue and to the associated eigenvector. After convergence is reached,

$$\boldsymbol{\psi}_i = \boldsymbol{\phi}_i, \qquad \omega_i^2 = \lambda_i + \mu.$$

The convergence of the method can be greatly enhanced if the shift μ is updated every few steps during the iterative procedure using the current best estimate of λ_i,

$$\lambda_{i,n+1} = \frac{\hat{\mathbf{x}}_{n+1}\mathbf{M}\,\mathbf{x}_n}{\hat{\mathbf{x}}_{n+1}\mathbf{M}\,\hat{\mathbf{x}}_{n+1}},$$

to improve the modified stiffness matrix to be used in the following iterations,

$$\overline{\mathbf{K}} = \overline{\mathbf{K}} - \lambda_{i,n+1}\mathbf{M}$$

Much thought was spent on the problem of choosing the initial shifts, so that all the eigenvectors can be computed in sequence without missing any of them.

Rayleigh Quotient for Discrete Systems

The matrix iteration procedures are usually used in conjunction with methods derived from the Rayleigh Quotient method.
The Rayleigh Quotient method was introduced using distributed flexibilty systems and an assumed shape function, but we have seen also an example where the Rayleigh Quotient was computed for a discrete system using an assumed shape vector.
The procedure to be used for discrete systems can be summarized as

$$x(t) = \phi Z_0 \sin\omega t, \qquad \dot{x}(t) = \omega\phi Z_0 \cos\omega t,$$

$$2T_{max} = \omega^2 \phi^T \mathbf{M}\,\phi, \qquad 2V_{max} = \phi^T \mathbf{K}\,\phi,$$

equating the maxima, we have

$$\omega^2 = \frac{\phi^T \mathbf{K}\,\phi}{\phi^T \mathbf{M}\,\phi} = \frac{k^\star}{m^\star},$$

where ϕ is an assumed shape vector, not an eigenvector.

Ritz Coordinates

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Rayleigh-Ritz Method

For a N *DOF* system, an *approximation* to a displacement vector x can be written in terms of a set of $M < N$ assumed shape, linearly independent vectors,

$$\phi_i, \quad i = 1, \ldots, M < N$$

and a set of *Ritz coordinates* z_i, $i - 1, \ldots, M < N$:

$$x = \sum_i \phi_i z_i = \Phi\, z.$$

We say *approximation* because a linear combination of $M < N$ vectors cannot describe every point in a N-space.

Rayleigh Quotient in Ritz Coordinates

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We can write the Rayleigh quotient as a function of the Ritz coordinates,

$$\omega^2(z) = \frac{z^T \Phi^T \mathbf{K}\,\Phi z}{z^T \phi^T \mathbf{M}\,\phi z} = \frac{\overline{k}(z)}{\overline{m}(z)},$$

but this is not an explicit function for any modal frequency...

On the other hand, we have seen that frequency estimates are always greater than true frequencies, so our best estimates are the the local minima of $\omega^2(z)$, or the points where all the derivatives of $\omega^2(z)$ with respect to z_i are zero:

$$\frac{\partial\omega^2(z)}{\partial z_j} = \frac{\overline{m}(z)\dfrac{\partial\overline{k}(z)}{\partial z_i} - \overline{k}(z)\dfrac{\partial\overline{m}(z)}{\partial z_i}}{(\overline{m}(z))^2} = 0, \qquad \text{for } i = 1, \ldots, M < N$$

Rayleigh Quotient in Ritz Coordinates

Observing that

$$\bar{k}(z) = \omega^2(z)\bar{m}(z)$$

we can substitute into and simplify the preceding equation,

$$\frac{\partial \bar{k}(z)}{\partial z_i} - \omega^2(z)\frac{\partial \bar{m}(z)}{\partial z_i} = 0, \qquad \text{for } i = 1, \ldots, M < N$$

With the positions

$$\overline{\mathbf{K}} = \mathbf{\Phi}^T \mathbf{K}\,\mathbf{\Phi}, \qquad ,\overline{\mathbf{M}} = \mathbf{\Phi}^T \mathbf{M}\,\mathbf{\Phi}$$

we have

$$\bar{k}(z) = \mathbf{z}^T\overline{\mathbf{K}}\mathbf{z} = \sum_i \sum_j \bar{k}_{ij} z_j z_i,$$

hence

$$\left\{\frac{\partial \bar{k}(z)}{\partial z_i}\right\} = \left\{2\sum_j \bar{k}_{ij} z_j\right\} = 2\overline{\mathbf{K}}\mathbf{z},$$

and, analogously

$$\left\{\frac{\partial \bar{m}(z)}{\partial z_i}\right\} = 2\overline{\mathbf{M}}\mathbf{z}.$$

Reduced Eigenproblem

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Substituting these results in $\frac{\partial \bar{k}(z)}{\partial z_i} - \omega^2(z)\frac{\partial \bar{m}(z)}{\partial z_i} = 0$ we can write a *new eigenvector problem*, in the M *DOF* Ritz coordinates space, with reduced $M \times M$ matrices:

$$\overline{\mathbf{K}}\,\mathbf{z} - \omega^2\overline{\mathbf{M}}\,\mathbf{z} = 0.$$

Modal Superposition?

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After solving the reduced eigenproblem, we have a set of M eigenvalues $\bar{\omega}_i^2$ and a corresponding set of M eigenvectors $\bar{z}_i$. What is the relation between these results and the eigenpairs of the original problem?
The $\bar{\omega}_i^2$ clearly are approximations from above to the real eigenvalues, and if we write $\bar{\psi}_i = \mathbf{\Phi}\bar{z}_i$ we see that, being

$$\bar{\psi}_i^T \mathbf{M} \bar{\psi}_j = \bar{z}_i^T \underbrace{\mathbf{\Phi}^T \mathbf{M} \mathbf{\Phi}}_{\overline{\mathbf{M}}} \bar{z}_j = \overline{M}_i \delta_{ij},$$

the approximated eigenvectors $\bar{\psi}_i$ are orthogonal with respect to the structural matrices and can be used in ordinary modal superposition techniques.

A Last Question

One last question: how many $\overline{\omega}_i^2$ and $\overline{\boldsymbol{\psi}}_i$ are *effective* approximations to the true eigenpairs? Experience tells that an effective approximation is to be expected for the first $M/2$ eigenthings.