Analysis of free vibrations

Analysis of free and forced vibrations

ME473 Dynamic finite element analysis of structures

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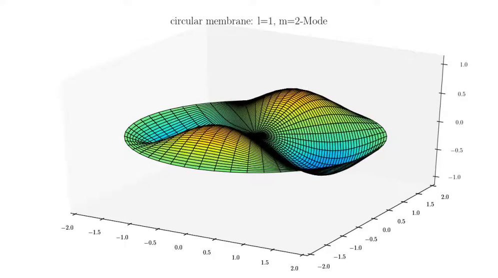
2025



Where do we stand?

Week	Module	Lecture topic	Mini-projects
1	Linear elastodynamics	Strong and weak forms	
2		Galerkin method	
3		Finite element method	Groups formation
4		Systematization of the procedure	Project 1 statement
5		3d elements, numerical integration	
6	Special structural elements	Bars and trusses	
7		Planar beams	Project 1 submission
8		Frames and grids	Project 2 statement
9		Kirchhoff-Love plates	
10		Reissner-Mindlin plates	
11		Shells	Project 2 submission
12	Free and forced vibrations	Analysis of free vibrations	Project 3 statement
13		Analysis of free vibrations	

Summary

- Recap week 12
- Numerical modal extraction algorithms for conservative systems
- Rayleigh's quotient
- Inverse iteration algorithm
- Subspace algorithm

Recommended readings

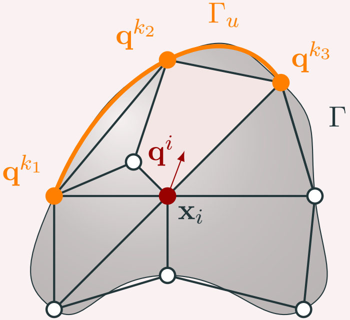
(B) Bathe, Finite Element Procedures in Engineering Analysis (chap. 10 and 11)
(P) Petyt, Introduction to finite element vibration analysis (chap. 11)
(G) Gmür, Dynamique des structures (§4.1 and §4.2)
(H) Hughes, The finite element method (chap. 10)

Recap week 12

Free vibrations of non-rotating conservative systems

The discretization of linear three-dimensional elastodynamics, as well as the analysis of vibrations in beams and plates via FEM, all lead to a system of ODE:

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{r}(t),$$



Free vibration: no external forcing is applied, i.e. $\mathbf{r}(t) = \mathbf{0}$.

- Generalized nodal displacements:

$$\mathbf{q}(t) = [\mathbf{q}^1(t), \dots, \mathbf{q}^n(t)]^T.$$

- **Boundary conditions:** $\mathbf{q}^k = \hat{\mathbf{q}}^k$ for all k such that $\mathbf{x}_k \in \Gamma_u$.
- **Initial conditions:** $\mathbf{q}(0) = \mathbf{u}_0$ and $\dot{\mathbf{q}}(0) = \mathbf{v}_0$

Free undamped discrete vibration problem:

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{0}$$

↓

Ansatz:

$$\mathbf{q}(t) = \alpha \mathbf{p} \cos(\omega t + \varphi)$$

↓

Generalized eigenvalue problem:

$$(\mathbf{K} - \omega^2 \mathbf{M})\mathbf{p} = 0$$

Solving the eigenvalue problem:

$$n = \dim(\mathbf{K}) = \dim(\mathbf{M})$$

There are n eigenvalues λ_j and n corresponding eigenvectors $\mathbf{p}_j$ such that:

Eigenvalues (*natural frequencies* squared): $\lambda_j = \omega_j^2$ are the roots of the characteristic polynomial:

$$\det(\mathbf{K} - \lambda \mathbf{M}) = 0.$$

Eigenvectors (*modal shapes*): $\mathbf{p}_j$ are the solution of the equation

$$(\mathbf{K} - \lambda_j \mathbf{M})\mathbf{p}_j = \mathbf{0}.$$

Rigid body modes

In the semi-discrete weak form obtained via finite element discretization:

- The **mass matrix M** is symmetric and strictly positive definite.
- The **stiffness matrix K** is symmetric and positive semi-definite:

$$\mathbf{K}\mathbf{p} = \mathbf{0} \quad \text{for certain nonzero vectors } \mathbf{p}.$$

Consequently, the eigenvalues λ_j of the generalized eigenvalue problem are all real and non-negative:

$$0 \leq \omega_1 \leq \omega_2 \leq \cdots \leq \omega_n.$$

Rigid body modes: zero eigenvalues (i.e., $\omega_j = 0$) correspond to *rigid body motions*, where the system undergoes displacement without internal deformation.

Orthonormalization of mode shapes

Let $\mathbf{p}_i$ and $\mathbf{p}_j$ two eigenvectors corresponding to the eigenvalues λ_i and λ_j, then

$$\mathbf{p}_i^T \mathbf{M} \mathbf{p}_j = \delta_{ij} \qquad \text{and} \qquad \mathbf{p}_i^T \mathbf{K} \mathbf{p}_j = \omega_i^2 \delta_{ij}$$

where δ_{ij} represent Kronecker symbol.

Consequences: if we organize the modal vectors $\mathbf{p}_i$ in a so-called modal matrix $\mathbf{P}$:

$$\mathbf{P} = \left[\begin{array}{c:c:c:c} \mathbf{p}_1 & \mathbf{p}_2 & \dots & \mathbf{p}_n \end{array}\right]$$

then

$$\mathbf{P}^T \mathbf{M} \mathbf{P} = \mathbf{I} \qquad \text{and} \qquad \mathbf{P}^T \mathbf{K} \mathbf{P} = \mathbf{\Lambda}$$

where $\mathbf{I}$ is the identity matrix of order n and $\mathbf{\Lambda}$ the *spectral matrix*:

$$\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \dots, \lambda_n) = \operatorname{diag}(\omega_1^2, \dots, \omega_n^2).$$

Numerical modal extraction algorithms

Transformation to standard form by inversion

Generalized eigenvalue problem

$$(\mathbf{K} - \lambda \mathbf{M})\mathbf{p} = \mathbf{0}$$

$\det \mathbf{M} \neq 0$

Standard eigenvalue problem

$$(\mathbf{A} - \lambda \mathbf{I})\mathbf{p} = \mathbf{0}$$

$\mathbf{A} = \mathbf{M}^{-1}\mathbf{K}$ dynamic stiffness matrix

$\det \mathbf{K} \neq 0$

Standard eigenvalue problem

$$(\mathbf{A} - \theta \mathbf{I})\mathbf{p} = \mathbf{0}$$

$\mathbf{A} = \mathbf{K}^{-1}\mathbf{M}$ dynamic flexibility matrix

$\theta = 1/\lambda$

The matrices $\mathbf{M}^{-1}\mathbf{K}$ and $\mathbf{K}^{-1}\mathbf{M}$ are not symmetric.

Transformation to standard form by decomposition

To reduce to a standard eigenvalue problem:

- Let $\mathbf{L}$ be the *Cholesky factor* of $\mathbf{M}$: $\mathbf{M} = \mathbf{L}\mathbf{L}^T$.

Since $\mathbf{M}$ is symmetric positive-definite, $\mathbf{L}$ is a real lower triangular matrix with positive diagonal entries.

- Define the change of variables $\mathbf{v} = \mathbf{L}^T\mathbf{p}$. Substituting into the original problem and multiplying by $\mathbf{L}^{-1}$ yields:

$$(\mathbf{K} - \omega^2\mathbf{L}\mathbf{L}^T)\mathbf{p} = 0 \quad \Rightarrow \quad (\mathbf{L}^{-1}\mathbf{K}\mathbf{L}^{-T} - \omega^2\mathbf{I})\mathbf{v} = 0.$$

- Standard eigenvalue problem for symmetric and positive definite matrix $\mathbf{A} = \mathbf{L}^{-1}\mathbf{K}\mathbf{L}^{-T}$:

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}.$$

The eigenvalues or the standard problem are the same as those of the generalized problem, and the eigenvectors are related by $\mathbf{p} = \mathbf{L}^{-T}\mathbf{v}$.

Transformation to standard form by decomposition

- Cholesky decomposition can be applied to $\mathbf{K}$ as well, since $\mathbf{K}$ is symmetric positive-definite:
$$\mathbf{K} = \mathbf{L}\mathbf{L}^T.$$
- Standard eigenvalue problem for symmetric and positive definite matrix $\mathbf{A} = \mathbf{L}^{-1}\mathbf{M}\mathbf{L}^{-T}$:
$$(\mathbf{A} - \theta\mathbf{I})\mathbf{v} = \mathbf{0}.$$

The eigenvalues or the standard problem are related to those of the generalized problem by $\theta = 1/\lambda$, and the eigenvectors are related by $\mathbf{p} = \mathbf{L}^{-T}\mathbf{v}$.

Small and large scale problems

Economical computation algorithms for extracting $(\lambda_j, \mathbf{p}_j)$ for $1 \leq j \leq n_{modes}$ are required in practical applications, where $n_{modes} \ll n$ is the number of desired eigenpairs.

Small-scale problems

- system matrices are of modest size $n \leq 250$ or $250 \leq n \leq 2500$ and small bandwidth matrices.
- An explicit reduction to standard eigenvalue form is typically employed:
  - *Generalized Jacobi method*
  - *Householder QR-algorithm*

Large-scale problems

- $n \geq 2500$.
- The most effective algorithms are:
  - *Subspace iteration method,*
  - *Lanczos' method,*
  - *Irons-Guyan reduction method,*
  - *Arnoldi method*
  - *Davidson method.*

Rayleigh's quotient

Definition and first properties

Let $\mathbf{w}$ be a vector in $\mathbb{R}^n$, the **Rayleigh's quotient** associated to the matrix pair $(\mathbf{K}, \mathbf{M})$ is defined as the scalar function:

$$\mathcal{R}(\mathbf{w}) = \frac{\mathbf{w}^T\mathbf{K}\mathbf{w}}{\mathbf{w}^T\mathbf{M}\mathbf{w}}$$

Properties

1. Homogeneity. Let α a non-zero constant, then

$$\mathcal{R}(\alpha\mathbf{w}) = \frac{(\alpha\mathbf{w})^T\mathbf{K}(\alpha\mathbf{w})}{(\alpha\mathbf{w})^T\mathbf{M}(\alpha\mathbf{w})} = \frac{\alpha^2\,\mathbf{w}^T\mathbf{K}\mathbf{w}}{\alpha^2\,\mathbf{w}^T\mathbf{M}\mathbf{w}} = \mathcal{R}(\mathbf{w})$$

2. Rayleigh quotient of an eigenvector:

$$\mathcal{R}(\mathbf{w} = \mathbf{p}_i) = \frac{\mathbf{p}_i^T\mathbf{K}\mathbf{p}_i}{\mathbf{p}_i^T\mathbf{M}\mathbf{p}_i} = \lambda_i = \omega_i^2$$

Stationarity of Rayleigh's quotient

First variation of Rayleigh's quotient:

$$\delta\mathcal{R}(\mathbf{w}) = \frac{2(\boldsymbol{\delta}\mathbf{w}^T\mathbf{K}\mathbf{w})(\mathbf{w}^T\mathbf{M}\mathbf{w}) - 2(\mathbf{w}^T\mathbf{K}\mathbf{w})(\boldsymbol{\delta}\mathbf{w}^T\mathbf{M}\mathbf{w})}{(\mathbf{w}^T\mathbf{M}\mathbf{w})^2}$$

$$= \frac{2\,\boldsymbol{\delta}\mathbf{w}^T}{\mathbf{w}^T\mathbf{M}\mathbf{w}}\left(\mathbf{K}\mathbf{w} - \frac{\mathbf{w}^T\mathbf{K}\mathbf{w}}{\mathbf{w}^T\mathbf{M}\mathbf{w}}\mathbf{M}\mathbf{w}\right)$$

$$= \frac{2\,\boldsymbol{\delta}\mathbf{w}^T}{\mathbf{w}^T\mathbf{M}\mathbf{w}}(\mathbf{K} - \mathcal{R}(\mathbf{w})\mathbf{M})\mathbf{w}$$

Stationary Rayleigh's quotient in the vicinity of an modal shape !

If $\mathbf{w} = \mathbf{p}_i$ then

$$(\mathbf{K} - \mathcal{R}(\mathbf{w})\mathbf{M})\mathbf{w} = (\mathbf{K} - \lambda_i\mathbf{M})\mathbf{p}_i = 0$$

Rayleigh principle

Modal expansion:

$$\mathbf{w} = z_1\mathbf{p}_1 + z_2\mathbf{p}_2 + \cdots + z_i\mathbf{p}_i + \cdots + z_n\mathbf{p}_n = \mathbf{P}\mathbf{z}$$

where

$$\mathbf{P} = [\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_i, \ldots, \mathbf{p}_n] \quad \text{modal matrix}$$
$$\mathbf{z} = [z_1, z_2, \ldots, z_i, \ldots, z_n]^T \quad \text{coefficient vector}$$

Then

$$\mathcal{R}(\mathbf{w} = \mathbf{P}\mathbf{z}) = \frac{\mathbf{z}^T\mathbf{P}^T\mathbf{K}\mathbf{P}\mathbf{z}}{\mathbf{z}^T\mathbf{P}^T\mathbf{M}\mathbf{P}\mathbf{z}} = \frac{\mathbf{z}^T\mathbf{\Lambda}\mathbf{z}}{\mathbf{z}^T\mathbf{z}} = \frac{\sum_{i=1}^n \lambda_i z_i^2}{\sum_{i=1}^n z_i^2}$$

If, without loss of generality, we impose $\mathbf{w}^T\mathbf{M}\mathbf{w} = 1$, then $\mathbf{z}^T\mathbf{z} = \sum_{i=1}^n z_i^2 = 1$ and

$$\mathcal{R}(\mathbf{w} = \mathbf{P}\mathbf{z}) = \sum_{i=1}^n \lambda_i z_i^2$$

Rayleigh principle (continued)

Let us consider an eigenvalue λ_j, then we can rewrite the Rayleigh's quotient as:

$$\mathcal{R}(\mathbf{w}) = \sum_{i=1}^{n} \lambda_i z_i^2 = \lambda_j - \lambda_j + \sum_{i=1}^{n} \lambda_i z_i^2 = \lambda_j - \lambda_j \left(\sum_{i=1}^{n} z_i^2 \right) + \sum_{i=1}^{n} \lambda_i z_i^2$$

$$= \lambda_j + \sum_{i=1}^{n} (\lambda_i - \lambda_j) z_i^2$$

With eigenvalues ordered as $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_i \leq \cdots \leq \lambda_n$, we have:

- If $j = 1$, then $\lambda_i - \lambda_1 \geq 0$ for all i, hence

$$\mathcal{R}(\mathbf{w}) = \lambda_1 + \sum_{i=1}^{n} (\lambda_i - \lambda_1) z_i^2 \geq \lambda_1.$$

- If $j = n$, then $\lambda_i - \lambda_n \leq 0$ for all i, hence

$$\mathcal{R}(\mathbf{w}) = \lambda_n + \sum^{n} (\lambda_i - \lambda_n) z_i^2 \leq \lambda_n.$$

Rayleigh quotient bounding theorem

- **Courant-Fischer formulas:**

$$\mathcal{R}(\mathbf{w}) \geq \lambda_1 = \min_{\mathbf{w}} \mathcal{R}(\mathbf{w})$$

$$\mathcal{R}(\mathbf{w}) \leq \lambda_n = \max_{\mathbf{w}} \mathcal{R}(\mathbf{w})$$

- **Bounding theorem:**

$$\lambda_1 \leq \mathcal{R}(\mathbf{w}) \leq \lambda_n$$

Modal frequencies and shapes search via Rayleigh quotient minimization

(1) Find λ_1 by minimization:

$$\lambda_1 = \min_{\mathbf{w}} \mathcal{R}(\mathbf{w})$$

(2) Find $\mathbf{p}_1$ by solving $(\mathbf{K} - \lambda_1 \mathbf{M})\mathbf{p}_1 = 0$.

(3) Find λ_2 by minimization:

$$\lambda_2 = \min_{\mathbf{w}} [\mathcal{R}(\mathbf{w});\ \mathbf{w}^T \mathbf{M} \mathbf{p}_1 = 0]$$

(4) Find $\mathbf{p}_2$ by solving $(\mathbf{K} - \lambda_2 \mathbf{M})\mathbf{p}_2 = 0$.

$$\vdots$$

(j) Find λ_j by minimization:

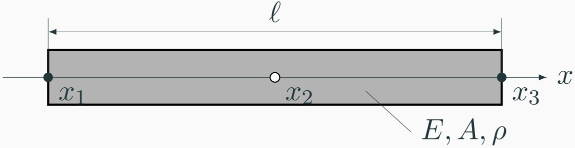
$$\lambda_j = \min_{\mathbf{w}} [\mathcal{R}(\mathbf{w});\ \mathbf{w}^T \mathbf{M} \mathbf{p}_i = 0,\ i = 1, 2, \ldots, j-1]$$

(j+1) Find $\mathbf{p}_j$ by solving $(\mathbf{K} - \lambda_j \mathbf{M})\mathbf{p}_j = 0$.

Example: Longitudinal vibrations of a free-free bar

Rayleigh quotient for longitudinal vibrations of free-free bar

Consider a free-free bar discretized by one bilinear element.



- ℓ length
- A cross-sectional area
- E Young's modulus
- ρ material density

Objective:
Compute the approximated natural frequencies and corresponding mode shapes via the minimization of Rayleigh's quotient

MATLAB example - longitudinal vibrations of free-free bar

Go to Matlab Drive

Rayleigh-Ritz analysis

Rayleigh-Ritz analysis: fundamentals

Goal: approximate the lowest n_{modes} eigenvalues and corresponding eigenvectors of the generalized eigenproblem $\mathbf{Kp} = \lambda\mathbf{Mp}$

Inputs:

- $\mathbf{K}$, $\mathbf{M}$: positive definite stiffness and mass matrices (or shifted to be so). If $\mathbf{K}$ is singular, use shift: set $\mathbf{K}_\sigma = \mathbf{K} + \sigma\mathbf{M}$ with $\sigma > 0$.
- n_{modes} linearly independent **Ritz basis vectors** $\boldsymbol{\psi}_i$, spanning a subspace $\mathcal{S}$.

Output:

- Approximated modal matrix of size $n \times n_{modes}$

$$\mathbf{P} = [\mathbf{p}_1, \ldots, \mathbf{p}_{n_{modes}}]$$

- Approximated spectral matrix:

$$\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_{n_{modes}})$$

Rayleigh-Ritz reduction algorithm

1. Any trial vector in $\mathcal{S}$ is written as $\mathbf{w} = \sum_{i=1}^{n_{modes}} x_i \boldsymbol{\psi}_i$, with coordinates x_i.
2. Insert $\mathbf{w} = \boldsymbol{\Psi}\mathbf{x}$ into $\mathcal{R}(\mathbf{w})$ to obtain the projected stiffness and mass matrices into the Ritz basis:

$$\tilde{\mathbf{K}} = \boldsymbol{\Psi}^T \mathbf{K} \boldsymbol{\Psi}, \qquad \tilde{\mathbf{M}} = \boldsymbol{\Psi}^T \mathbf{M} \boldsymbol{\Psi},$$

   where $\boldsymbol{\Psi} = [\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \dots, \boldsymbol{\psi}_{n_{modes}}]$.
3. Solve the reduced $(n_{modes} \times n_{modes})$ generalized eigenvalue problem by minimization:

$$\tilde{\mathbf{K}}\mathbf{x} = \phi\, \tilde{\mathbf{M}}\mathbf{x}.$$

   to obtain approximate eigenpairs $(\phi_i, \mathbf{x}_i)$ for $i = 1, 2, \dots, n_{modes}$.
4. Compute the modal and the spectral matrices:

$$\tilde{\boldsymbol{\Lambda}} = \mathrm{diag}(\phi_1, \phi_2, \dots, \phi_{n_{modes}}),$$

   and the approximate mode shapes

$$\mathbf{p}_i = \boldsymbol{\Psi}\mathbf{x}_i.$$

Practical aspects and remarks

Upper-bound property:

$$\lambda_i \leq \phi_i, \qquad i = 1, \ldots, n_{modes}.$$

- Ritz basis often obtained from static solutions:

$$\mathbf{K}\Psi = \mathbf{R},$$

  where $\mathbf{R}$ contains chosen load patterns.
- Accuracy depends on how well $\mathcal{S}$ approximates the subspace of the lowest eigenmodes.
- Many well-known methods are special cases of Rayleigh–Ritz:
  - **Static condensation** (Irons-Guyan reduction)
  - **Component mode synthesis**
  - **Subspace iteration**

Inverse iteration algorithm

General idea of inverse and forward iteration

Goal: compute **one** eigenvector of the generalized eigenproblem $\mathbf{K}\mathbf{p} = \lambda\mathbf{M}\mathbf{p}$.

Idea: Use an *iterative* improvement of an assumed eigenvector.

- Start from an arbitrary vector $\mathbf{p}^{(0)}$.
- Generate a sequence of vectors $\mathbf{p}^{(1)}, \mathbf{p}^{(2)}, \ldots$ that converge to an eigenvector.
- Compute an approximate eigenvalue using Rayleigh's quotient:

$$\lambda^{(k)} = \mathcal{R}(\mathbf{p}^{(k)}).$$

Inverse iteration:

- Form a *"force"* vector: $\mathbf{R}_1 = \mathbf{M}\mathbf{p}^{(0)}$.
- Solve the static-like equilibrium problem:
$$\mathbf{K}\mathbf{p}^{(1)} = \mathbf{R}_1,$$
- Repeat until convergence is met.

Forward iteration:

- Compute $\mathbf{R}_1 = \mathbf{K}\mathbf{p}^{(0)}$.
- Solve
$$\mathbf{M}\mathbf{p}^{(1)} = \mathbf{R}_1,$$
- Repeat until convergence is met.

Inverse iteration algorithm

Inputs:

- $\mathbf{K}$, $\mathbf{M}$: stiffness and mass matrices
- $\mathbf{p}^{(0)}$: initial guess vector (non-zero)
- σ: spectral shift
- ε: convergence tolerance

Algorithm:

1. If $\mathbf{K}$ is singular, use shift: set $\mathbf{K}_\sigma = \mathbf{K} + \sigma\mathbf{M}$
2. For $k = 1, 2, \ldots$ until convergence:
   - Solve for $\bar{\mathbf{p}}^{(k)}$ the static equilibrium problem

     $$\mathbf{K}_\sigma\,\bar{\mathbf{p}}^{(k)} = \mathbf{M}\,\mathbf{p}^{(k-1)}$$

   - $\mathbf{M}$-normalize the vector $\bar{\mathbf{p}}^{(k)}$:

     $$\mathbf{p}^{(k)} = \bar{\mathbf{p}}^{(k)} / \sqrt{(\bar{\mathbf{p}}^{(k)})^T\mathbf{M}\bar{\mathbf{p}}^{(k)}}$$

   - Check convergence: $\|\mathbf{p}^{(k)} - \mathbf{p}^{(k-1)}\| < \varepsilon$

Output: approximated eigenvector $\mathbf{p}^{(k)}$ and eigenvalue $\lambda^{(k)} = \mathcal{R}(\mathbf{p}^{(k)}) - \sigma$.

Convergence of inverse iteration

- The inverse iteration converges to $\mathbf{p}_j$, the eigenvector associated with the eigenvalue closest to σ, if the initial guess $\mathbf{p}^{(0)}$ is not $\mathbf{M}$-orthogonal to $\mathbf{p}_j$.
- If no shift is used, i.e. $\sigma = 0$, the method converges to the eigenvector associated with the *smallest eigenvalue* provided the orthogonality condition on the initial guess is met.

- The rate of convergence depends on the ratio

$$\rho = \frac{|\lambda_j - \sigma|}{|\lambda_{j+1} - \sigma|},$$

where λ_j is the eigenvalue closest to σ and λ_{j+1} is the next closest eigenvalue.
- If $\varepsilon = 10^{-2s}$, then approximately $2s$ correct digits of the eigenvector are obtained and s correct digits of the eigenvalue.

Subspace iteration method

General ideas behind the subspace iteration method

Goal: compute the lowest $n_{modes} \ll n$ eigenpairs $(\mathbf{p}_i, \lambda_i)$ of the generalized eigenproblem

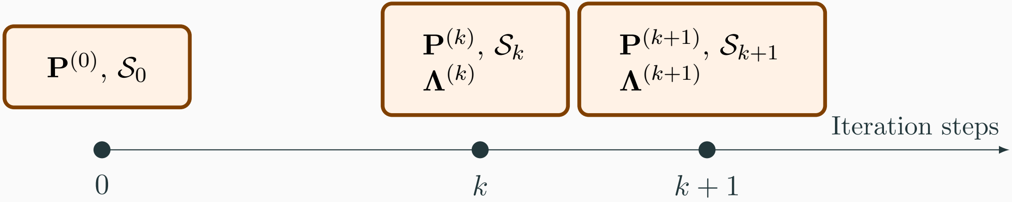
$$\mathbf{K}\mathbf{p} = \lambda \mathbf{M}\mathbf{p}.$$

Method developed and named by K. J. Bathe consists of the following three steps:

1. Establish q starting iteration vectors, $q > n_{modes}$, where n_{modes} is the number of eigenvalues and vectors to be calculated.
2. Use **inverse iteration** on the q vectors and **Rayleigh-Ritz analysis** to extract the "*best*" eigenvalue and eigenvector approximations from the q iteration vectors.
3. After iteration convergence, use the **Sturm sequence** check to verify that the required eigenvalues and corresponding eigenvectors have been calculated.

Preliminary considerations

Named the subspace iteration method because the iteration is equivalent to iterating with a q-dimensional subspace $\mathcal{S}_k = \text{span}(\mathbf{p}_1^{(k)}, \ldots, \mathbf{p}_q^{(k)})$ and should not be regarded as a simultaneous iteration with q individual iteration vectors.



The effectiveness of the algorithm lies in that it is much easier to establish a q-dimensional starting subspace which is close to $\text{span}(\mathbf{p}_1, \ldots, \mathbf{p}_{n_{modes}})$ than to find n_{modes} vectors that are each close to a required eigenvector $\mathbf{p}_i$.

Preliminary considerations

- All characteristics of the Ritz analysis pertain also to the subspace iteration; i.e., the smallest eigenvalues are approximated best in the iteration, and all eigenvalue approximations are **upper bounds** on the actual eigenvalues sought.
- Because the iteration is performed on a subspace, **convergence of the subspace** is all that is required and not convergence of individual iteration vectors to eigenvectors.
- If the initial vectors are linear combinations of the required eigenvectors, the solution algorithm converges in one step.

Pseudo-code of the subspace iteration method

Inputs:

- $\mathbf{K}$, $\mathbf{M}$: stiffness and mass matrices of dimension $n \times n$.
- n_{modes}: number of desired eigenmodes.
- q: number of iteration vectors, with $q > n_{modes}$.
- $\mathbf{P}^{(0)} \in \mathbb{R}^{n \times q}$: initial guess matrix of linearly independent vectors

$$\mathbf{P}^{(0)} = [\mathbf{p}_1^{(0)}, \ldots, \mathbf{p}_q^{(0)}]$$

- σ: spectral shift (optional)
- ε: convergence tolerance

Output:

- Approximated eigenvectors: $\mathbf{P}^{(k)} = [\mathbf{p}_1^{(k)}, \ldots, \mathbf{p}_q^{(k)}]$
- Approximated eigenvalues: $\mathbf{\Lambda}^{(k)} = \mathrm{diag}(\lambda_1^{(k)}, \ldots, \lambda_q^{(k)})$

Pseudo-code of the subspace iteration method

Algorithm:

1. If $\mathbf{K}$ is singular, use shift: set $\mathbf{K}_\sigma = \mathbf{K} + \sigma\mathbf{M}$
2. For $k = 1, 2, \ldots$ until convergence:
   - Do step 1: perform inverse iteration on q vectors to obtain
   $$\overline{\mathbf{P}^{(k)}}.$$
   - Do step 2a: compute the projected stiffness and mass matrices:
   $$\mathbf{K}^{(k)} \qquad \text{and} \qquad \mathbf{M}^{(k)}.$$
   - Do step 2b: solve the projected generalized eigenvalue problem to obtain the projected modal matrix and the spectral matrix:
   $$\mathbf{Z}^{(k)} \qquad \text{and} \qquad \mathbf{\Lambda}^{(k)}.$$
   - Do step 2c: calculate the updated modal matrix $\mathbf{P}^{(k)}$.
   - Do step 3: check convergence

Subspace iteration steps

1. **Step 1:** Inverse iteration on q vectors: find the $(n \times q)$ matrix $\overline{\mathbf{P}^{(k)}}$ such that

$$\mathbf{K}\overline{\mathbf{P}^{(k)}} = \mathbf{M}\mathbf{P}^{(k-1)}$$

2. **Step 2a:** Compute projected stiffness and mass matrices $(q \times q)$:

$$\mathbf{K}^{(k)} = (\overline{\mathbf{P}^{(k)}})^T \mathbf{K}\overline{\mathbf{P}^{(k)}}, \quad \mathbf{M}^{(k)} = (\overline{\mathbf{P}^{(k)}})^T \mathbf{M}\overline{\mathbf{P}^{(k)}}$$

3. **Step 2b:** Solve $(q \times q)$ generalized eigenvalue problem: Find the projected modal matrix $\mathbf{Z}^{(k)}$ and the spectral matrix $\mathbf{\Lambda}^{(k)}$ such that

$$\mathbf{K}^{(k)}\mathbf{Z}^{(k)} = \mathbf{M}^{(k)}\mathbf{Z}^{(k)}\mathbf{\Lambda}^{(k)}$$

4. **Step 2c:** Calculate the updated modal matrix $(n \times q)$:

$$\mathbf{P}^{(k)} = \overline{\mathbf{P}^{(k)}}\mathbf{Z}^{(k)}$$

Step 1 - Inverse iteration on q vectors

Suppose that the Step 1 is replace by a simultaneous inverse iteration on m eigenvectors:

$$\mathbf{P}^{(k)} = (\mathbf{K}^{-1}\mathbf{M})\mathbf{P}^{(k-1)} = \cdots = (\mathbf{K}^{-1}\mathbf{M})^k\,\mathbf{P}^{(0)}$$

Define the subspace $\mathcal{S}^{(k)}$ of rank q, spanned by the vectors $\{\mathbf{p}_i^{(k)}\}$.
$\mathbf{P}^{(k)} = [\mathbf{p}_1^{(k)}, \ldots, \mathbf{p}_q^{(k)}]$ forms a *non-orthogonal* basis of $\mathcal{S}^{(k)}$.

- ✗ All columns of $\mathbf{P}^{(k)}$ tend toward $\mathbf{p}_1$
- ✗ Collinearity if no orthogonalization is applied !

Orthogonalization of vectors $\mathbf{p}_i^{(k)}$ at each iteration needed !

Modified Step 2 - Gram-Schmidt orthogonalization

1. **Step 1:** Inverse iteration on q vectors: find the $(n \times q)$ matrix $\overline{\mathbf{P}^{(k)}}$ such that

$$\mathbf{K}\overline{\mathbf{P}^{(k)}} = \mathbf{M}\mathbf{P}^{(k-1)}$$

2. **Step 2:** Grand-Schmidt orthogonalization:

$$\mathbf{P}^{(k+1)} = \mathbf{P}^{(k)}\mathbf{R}^{k}$$

where $\mathbf{R}^k$ is an upper triangular matrix chosen in such way that

$$(\mathbf{P}^{(k+1)})^T\mathbf{M}\mathbf{P}^{(k+1)} = \mathbf{I}$$

Gram-Schmidt method is inefficient as iteration vector $\mathbf{p}_i^{(k)}$ is forced to converge to a prescribed eigenvector $\mathbf{p}_i$ without allowing a more effective linear combination of the iteration vectors to take place.

Step 2 - Orthogonalization by minimization of the Rayleigh quotient

- Orthogonalization by minimization of the Rayleigh quotient:

$$\mathcal{R}(\mathbf{w}^{(k)}) = \frac{(\mathbf{w}^{(k)})^T \mathbf{K} \mathbf{w}^{(k)}}{(\mathbf{w}^{(k)})^T \mathbf{M} \mathbf{w}^{(k)}}$$

- Let $\mathbf{w}^{(k)} = \overline{\mathbf{P}^{(k)}} \mathbf{z}^{(k)}$
- Projected Rayleigh's quotient:

$$\mathcal{R}(\mathbf{w}^{(k)}) = \frac{(\mathbf{z}^{(k)})^T \mathbf{K}^{(k)} \mathbf{z}^{(k)}}{(\mathbf{z}^{(k)})^T \mathbf{M}^{(k)} \mathbf{z}^{(k)}}$$

where

$$\mathbf{K}^{(k)} = (\overline{\mathbf{P}^{(k)}})^T \mathbf{K} \overline{\mathbf{P}^{(k)}}, \quad \mathbf{M}^{(k)} = (\overline{\mathbf{P}^{(k)}})^T \mathbf{M} \overline{\mathbf{P}^{(k)}}$$

Step 2b - Solve projected generalized eigenvalue problem

- Minimization of the projected Rayleigh's quotient (generalized eigenvalue problem of dimension $q \times q$)
- Stationary condition:

$$\delta\mathcal{R}(\mathbf{w}^{(k)}) = 0 \qquad \Rightarrow \qquad \mathbf{K}^{(k)}\mathbf{z}^{(k)} = \lambda^{(k)}\mathbf{M}^{(k)}\mathbf{z}^{(k)}$$

- Solve via transformation method (e.g., Jacobi method):

$$\mathbf{K}^{(k)}\mathbf{Z}^{(k)} = \mathbf{M}^{(k)}\mathbf{Z}^{(k)}\mathbf{\Lambda}^{(k)}$$

- Ritz vectors and values:

$$\mathbf{Z}^{(k)} = [\mathbf{z}_1^{(k)}, \ldots, \mathbf{z}_q^{(k)}], \quad \text{and} \quad \mathbf{\Lambda}^{(k)} = \mathrm{diag}(\lambda_1^{(k)}, \ldots, \lambda_q^{(k)})$$

Step 2c - Update modal matrix and orthogonality check

- Update the modal matrix:

$$\mathbf{P}^{(k)} = \overline{\mathbf{P}^{(k)}}\mathbf{Z}^{(k)}$$

- Orthogonality check:

$$(\mathbf{P}^{(k)})^T\mathbf{M}\mathbf{P}^{(k)} = \mathbf{I}$$

Step 3 - Convergence to stop iteration

Convergence criterion based on relative change of eigenvalues:

$$\frac{|\lambda_i^{(k)} - \lambda_i^{(k-1)}|}{\lambda_i^{(k)}} < \varepsilon, \quad i = 1, 2, \ldots, n_{modes}$$

Starting iteration vectors $\mathbf{P}^{(0)}$

- The starting iteration vectors in $\mathbf{P}^{(0)}$ should not be too close to each other, i.e., they should be linearly independent.
- Higher convergence rate can be obtained by increasing q. However, using more iteration vectors will also increase the computer effort for one iteration. In practice

$$q = \min(2n_{modes}, n_{modes} + 8)$$

Empirical guidelines

- The first column of $\mathbf{P}^{(0)}$ should be the diagonal of $\mathbf{M}$. This ensures that all mass degrees of freedom are excited.
- The other columns in $\mathbf{P}^{(0)}$, except for the last column, should be unit vectors $\mathbf{e}_i$, with entries $+1$ at the degrees of freedom with the smallest ratios k_{ii}/m_{ii}, and the last column in $\mathbf{P}^{(0)}$ should be a random vector with values in $[0, 1]$.

Convergence of the subspace iteration method

- Iteration is performed with q vectors, $q > n_{modes}$, but convergence is measured only on the approximations obtained for the n_{modes} smallest eigenvalues.
- If the starting iteration vectors in $\mathbf{P}^{(0)}$, are not orthogonal to any one of the required eigenvectors $\mathbf{p}_1, \ldots, \mathbf{p}_{n_{modes}}$, then as $k \to \infty$

$$\tilde{\mathcal{S}}_k = \text{span}(\mathbf{p}_1^{(k)}, \ldots, \mathbf{p}_{n_{modes}}^{(k)}) \to \mathcal{S}_\infty = \text{span}(\mathbf{p}_1, \ldots, \mathbf{p}_{n_{modes}})$$

- Assuming that in the iteration the vectors in $\mathbf{P}^{(k+1)}$ are ordered in such way that the i-th diagonal element in $\mathbf{\Lambda}^{(k+1)}$ is larger than the $(i-1)$-st element for $i = 2, \ldots, p$, then the i-th column in $\mathbf{P}^{(k+1)}$ converges to $\mathbf{p}_i$ and the convergence rate is

$$\lambda_i / \lambda_{p+1}$$

  Although this is an asymptotic convergence rate, it indicates that the smallest eigenvalues converge fastest.

Final Sturm sequence check

After convergence is achieved, a final check based on the Sturm sequence property can be performed to ensure that the number of computed eigenvalues below a certain value is correct.

- The Sturm sequence property states that the number of eigenvalues of the generalized eigenvalue problem $\mathbf{Kp} = \lambda\mathbf{Mp}$ that are less than a given value λ^* is equal to the number of negative pivots obtained when performing an $\mathbf{LDL}^T$ factorization of the matrix $\mathbf{K} - \lambda^*\mathbf{M}$.
- This property can be used to verify that the number of computed eigenvalues below a certain threshold matches the expected count, providing an additional layer of validation for the results obtained from the subspace iteration method.