BENG 221: Mathematical Methods in Bioengineering

Lecture 3

Canonical LTI ODEs, Eigenmode Analysis, and Principal Component Analysis

References

http://en.wikipedia.org/wiki/LTI_system_theory

https://en.wikipedia.org/wiki/Eigenvalues_and_eigenvectors

https://en.wikipedia.org/wiki/Principal_component_analysis

https://en.wikipedia.org/wiki/Singular-value_decomposition

EIGEN ANALYSIS OF CANONICAL LTI ODES:

Canonical form:

$$\frac{d\vec{u}}{dt} = \underset{\text{MATRIX}}{\bar{\bar{A}}} \cdot \underset{\text{VECTOR}}{\vec{u}} + \vec{f} \quad \text{with} \quad \underset{\text{I.C.}}{\vec{u}(0) = \vec{u}_0}$$

Homogeneous case: $\vec{f} = 0$

$$\frac{d\vec{u}}{dt} = \bar{\bar{A}} \cdot \vec{u}$$

Trivial solution: $\vec{u}(t) \equiv 0$

Non-trivial solutions are the EIGENMODES $\vec{u}_i(t) \neq 0$

where in general $\vec{u}(t) = \sum_i c_i \vec{u}_i(t)$

These eigenmodes can be found by SEPARATION OF VARIABLES in terms of EIGENVECTORS and EIGENVALUES of $\bar{\bar{A}}$.

The general solution can also be found by Laplace in terms of the same eigen decomposition.

SEPARATION OF VARIABLES:

Try a non-trivial solution to the homogeneous ODE:

$$\frac{d\vec{u}}{dt} = \bar{\bar{A}} \cdot \vec{u}$$

of the form, separated in time and (vector) space:

$$\vec{u}(t) = \underbrace{\vec{U}}_{\substack{\text{VECTOR} \\ \text{(SPACE)} \\ \text{independent of} \\ \text{TIME}}} \cdot \underbrace{v(t)}_{\substack{\text{SCALAR} \\ \text{function of} \\ \text{TIME}}}$$

$$\Rightarrow \quad \frac{d}{dt}\left(\vec{U}\, v(t)\right) = \vec{U}\,\frac{dv}{dt} = \bar{\bar{A}} \cdot \vec{U}\, v(t)$$

This identity can only non-trivially hold when $\bar{\bar{A}} \cdot \vec{U}$ and $\vec{U}$ are co-linear:

$$\bar{\bar{A}} \cdot \vec{U} = \lambda \vec{U} \qquad \lambda \neq 0 \text{ (NON-TRIVIAL)}$$

i.e., $\vec{U}$ is an EIGENVECTOR of $\bar{\bar{A}}$ with EIGENVALUE λ.

$$\Rightarrow \quad \vec{U} \frac{dv}{dt} = \lambda \vec{U} v(t) \qquad \text{where } \|\vec{U}\| \neq 0 \text{ (NON-TRIVIAL)}$$

$$\Rightarrow \quad \frac{dv}{dt} = \lambda v \qquad \text{or} \qquad d(\ln v) = \lambda \, dt$$

$$\ln v = \lambda t + cst$$

$$v(t) = e^{\lambda t} \cdot \underbrace{e^{cst}}_{\text{another constant, } c}$$

$$v(t) = c \cdot e^{\lambda t}$$

$$\Rightarrow \quad \vec{u}(t) = \vec{U} e^{\lambda t}$$ is ONE solution to the homogeneous ODE where $\bar{\bar{A}} \cdot \vec{U} = \lambda \vec{U}$.

In general there are N such eigenvectors / eigenvalues:

$$\bar{\bar{A}} \cdot \vec{U}_i = \lambda_i \vec{U}_i \qquad i = 1, \dots N$$

each contributing such solution (EIGENMODE):

$$\vec{u}_i(t) = \vec{U}_i \cdot e^{\lambda_i t}$$

where N is the dimension of $\vec{u}$ (ORDER of the ODE).

The general solution is thus a superposition of EIGENMODES:

$$\vec{u}(t) = \sum_{i=1}^{N} c_i \, \vec{u}_i(t) = \sum_{i=1}^{N} c_i \, \vec{U}_i \, e^{\lambda_i t}$$

The particular solution (values of c_i) is determined by the INITIAL CONDITIONS (I.C.s):

$$\vec{u}_0 = \vec{u}(0) = \sum_{i=1}^{N} c_i \vec{u}_i(0) = \sum_{i=1}^{N} c_i \cdot \vec{U}_i$$

$\rightarrow$ N linear equations in the N unknown c_i's

SPECIAL CASE: for $\bar{\bar{A}}$ symmetric:

$\rightarrow$ the eigenvalues λ_i are REAL

$\rightarrow$ the eigenvectors $\vec{U}_i$ are ORTHOGONAL:
(ORTHONORMAL upon rescaling)

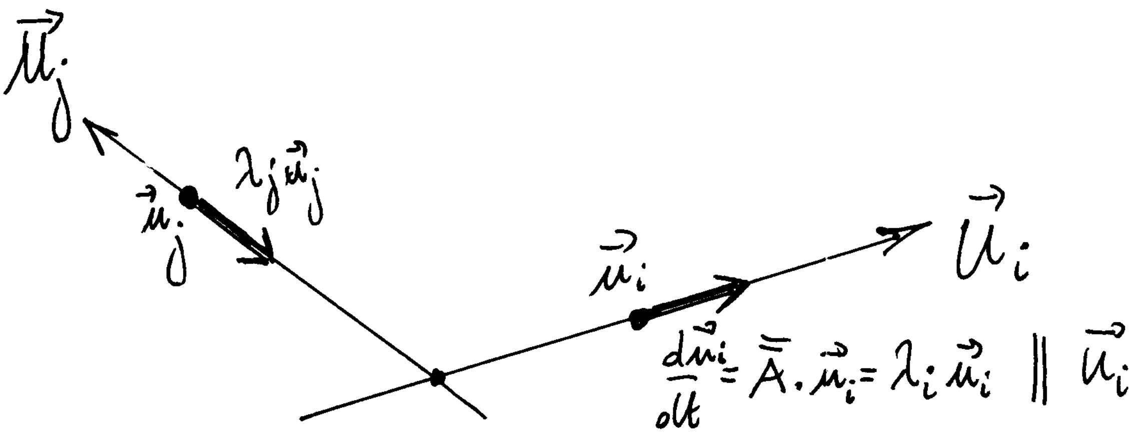
$$\vec{U}_i \cdot \vec{U}_j = \delta_{ij} = \begin{cases} 1 & \text{for } i=j \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow \quad c_i = \vec{u}_0 \cdot \vec{U}_i$$

$$\Rightarrow \quad \vec{u}(t) = \sum_{i=1}^{N} (\vec{u}_0 \cdot \vec{U}_i) \, \vec{U}_i \, e^{\lambda_i t}$$

EIGENVECTORS AS PRINCIPAL AXES:

The eigenvectors of $\bar{\bar{A}}$ are those directions in state space $\vec{u}$ for which the homogeneous dynamics is decoupled and self-contained:



Eigen decomposition and transformation to principal axes:

$$\bar{\bar{A}} = \bar{\bar{U}} \cdot \bar{\bar{\Lambda}} \cdot \bar{\bar{U}}^{-1}$$

with $\bar{\bar{U}} = \left(\vec{u}_1 \; \vec{u}_2 \; \ldots \; \vec{u}_n \right)$ eigenvector matrix

$$\bar{\bar{\Lambda}} = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix}$$ diagonal eigenvalue matrix

Equivalently: $\bar{\bar{A}} \cdot \bar{\bar{U}} = \bar{\bar{U}} \cdot \bar{\bar{\Lambda}}$ or $\bar{\bar{A}} \cdot \vec{u}_i = \lambda_i \vec{u}_i$

$$\frac{d\vec{u}}{dt} = \bar{\bar{A}} \cdot \vec{u} + \vec{f}$$

$$= \bar{\bar{U}} \cdot \bar{\bar{\Lambda}} \cdot \bar{\bar{U}}^{-1} \cdot \vec{u} + \vec{f}$$

$$\Downarrow$$

$$\bar{\bar{U}}^{-1} \frac{d\vec{u}}{dt} = \cancel{\bar{\bar{U}}^{-1}} \cdot \cancel{\bar{\bar{U}}} \cdot \bar{\bar{\Lambda}} \cdot \bar{\bar{U}}^{-1} \cdot \vec{u} + \bar{\bar{U}}^{-1} \cdot \vec{f}$$

$$\Downarrow$$

$$\frac{d\vec{u}'}{dt} = \bar{\bar{\Lambda}} \cdot \vec{u}' + \vec{f}'$$

where $\begin{cases} \vec{u}' = \bar{\bar{U}}^{-1} \cdot \vec{u} \\ \vec{f}' = \bar{\bar{U}}^{-1} \cdot \vec{f} \end{cases}$ projections onto principal axes $\bar{\bar{U}}$

$$\frac{du_i'}{dt} = \lambda_i u_i' + f_i'$$

$$u_i'(t) = \underbrace{u_i'(0) e^{\lambda_i t}}_{\text{I.C.}} + \int_0^t f_i'(\theta)\, e^{\lambda_i (t-\theta)}\, d\theta$$

I.C. ; DRIVING FORCE : projected on principal axis $\vec{U}_i$

and $\vec{u}(t) = \sum_i u_i'(t) \cdot \vec{U}_i$

$$\Rightarrow \vec{u}(t) = \sum_i u_i^?(0)\, e^{\lambda_i t} . \vec{U}_i + \sum_i \int_0^t f_i^?(\theta) e^{\lambda_i (t-\theta)} d\theta . \vec{U}_i$$

where : $\begin{cases} u_i^?(0) = \left(\bar{\bar{U}}^{-1} \vec{u}(0)\right)_i & : \text{PROJECTION OF I.C. } \vec{u}(0) \text{ ONTO PRINCIPAL AXIS } i \\ f_i^?(\theta) = \left(\bar{\bar{U}}^{-1} \vec{f}(\theta)\right)_i & : \text{PROJECTION OF STIMULUS } \vec{f}(\theta) \text{ ONTO PRINCIPAL AXIS } i \end{cases}$

Special case : $\bar{\bar{A}}$ = symmetric

$$\Rightarrow \bar{\bar{U}}^{-1} = \bar{\bar{U}}^T \quad (\text{and } \lambda_i = \text{real})$$

Then: $\begin{cases} u_i^?(0) = \vec{U}_i^T \vec{u}(0) = \vec{U}_i \bullet \vec{u}(0) \\ f_i^?(\theta) = \vec{U}_i^T \vec{f}(\theta) = \vec{U}_i \bullet \vec{f}(\theta) \end{cases}$ DOT PRODUCTS

And thus: $$\vec{u}(t) = \sum_i \left(\vec{U}_i \bullet \vec{u}(0)\right) e^{\lambda_i t} \vec{U}_i + \sum_i \int_0^t \left(\vec{U}_i \bullet \vec{f}(\theta)\right) e^{\lambda_i (t-\theta)} d\theta . \vec{U}_i$$

NOTES:

1) The characteristic equation $\det\left(\bar{\bar{A}} - \lambda \bar{\bar{I}}\right) = 0$ to find the eigenvalues $\lambda_1, \lambda_2, \dots \lambda_n$ is the SAME polynomial zero equality (denominator of Laplace transfer function) to find the poles $p_1, p_2, \dots p_n$, where $s = \lambda$:

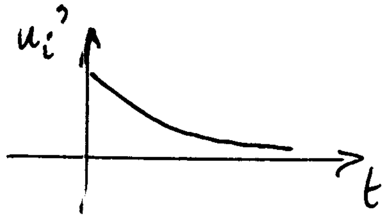
$$s \cdot \vec{U}(s) - \vec{u}(0) = \bar{\bar{A}} \cdot \vec{U}(s) + \vec{F}(s)$$

$$\left(s \bar{\bar{I}} - \bar{\bar{A}}\right) \cdot \vec{U}(s) = \vec{u}(0) + \vec{F}(s)$$

2) The dynamics is STABLE when all eigenvalues have negative real components:

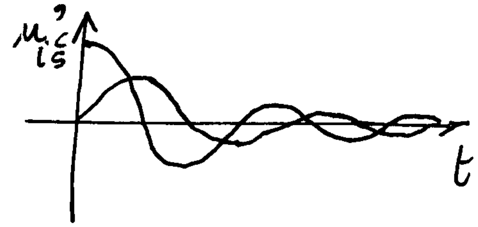
$$\mathrm{Re}(\lambda_i) \leq 0 \qquad \forall i$$

— REAL: $\lambda_i \leq 0$



— COMPLEX CONJUGATE PAIR:

$$\lambda_{i\pm} = -\sigma \pm j\omega$$



3) The eigenvalues with the LARGEST $Re(\lambda_i)$ dominate the dynamics $\vec{u}(t)$ in the long run ($t \to \infty$):

$$\vec{u} = \sum_i u_i^?(t) \cdot \vec{U}_i$$

$$= \sum_i \left(u_i^?(0)\, e^{\lambda_i t} + \int_0^t f_i^?(\theta)\, e^{\lambda_i (t-\theta)}\, d\theta \right) \cdot \vec{U}_i$$

I.C. DRIVING FORCE (finite)

$$\propto \quad e^{Re(\lambda_i).t} \cdot \vec{U}_i \quad \text{as } t \to \infty$$

for the largest $Re(\lambda_i)$

(< 0 if $\vec{u}$ is stable)

SINGULAR VALUE DECOMPOSITION (SVD) & PRINCIPAL COMPONENT ANALYSIS (PCA)

— SVD is an extension to eigen decomposition :

$$\overline{\overline{X}} = \overline{\overline{U}} \cdot \overline{\overline{\Sigma}} \cdot \overline{\overline{W}}^*$$

$(n \times p) \div (n \times n) \quad (n \times p) \quad (p \times p)$

- $\overline{\overline{X}} = \left(\vec{x}[1], \vec{x}[2], \dots \vec{x}[p] \right)$

  p points of process $\vec{x}$ in n-dimensional space

- $\overline{\overline{U}}$ and $\overline{\overline{W}}$ are orthogonal matrices

$$\overline{\overline{U}}^* \cdot \overline{\overline{U}} = \overline{\overline{I}} \ (n \times n)$$
$$\overline{\overline{W}}^* \cdot \overline{\overline{W}} = \overline{\overline{I}} \ (p \times p)$$

with $*$ the complex conjugate transpose

$\left(\overline{\overline{W}}^* = \overline{\overline{W}}^T \text{ when } \overline{\overline{X}} \text{ is real} \right)$

- $$\overline{\overline{\Sigma}} = \begin{pmatrix} \Sigma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \Sigma_2 & \ddots & & & & \\ 0 & 0 & \cdots & \Sigma_n & 0 & \cdots & 0 \end{pmatrix}$$ $(n \times p)$ diagonal matrix

with singular values $\Sigma_1, \Sigma_2, \dots \Sigma_n$
(real & positive)

— SVD is an efficient method for PCA :

$\overline{\overline{U}} = (\vec{u}_1, \vec{u}_2, \dots \vec{u}_n)$ are the principal axes of the data $\vec{x}[j]$ along which the covariance is diagonal :

$$\mathrm{cov}(\vec{x}) = \frac{1}{p} \sum_{j=1}^{p} \vec{x}[j] . \vec{x}^*[j]$$

$$= \frac{1}{p} \overline{\overline{X}} . \overline{\overline{X}}^*$$

$$= \frac{1}{p} (\overline{\overline{U}} . \overline{\overline{\Sigma}} . \cancel{\overline{\overline{W}}^*}) . (\cancel{\overline{\overline{W}}} . \overline{\overline{\Sigma}}^* . \overline{\overline{U}}^*)$$

$$= \frac{1}{p} \overline{\overline{U}} . (\overline{\overline{\Sigma}} . \overline{\overline{\Sigma}}^*) . \overline{\overline{U}}^* = \overline{\overline{U}} . \overline{\overline{C}} . \overline{\overline{U}}^*$$

with diagonal covariance $\overline{\overline{C}} = \frac{1}{p} \overline{\overline{\Sigma}} . \overline{\overline{\Sigma}}^*$

$$C_i = \frac{1}{p} (\Sigma_i)^2$$

The projections of $\vec{x}[j]$ onto the principal axes $\vec{U}_i$ are the PRINCIPAL COMPONENTS $T_i[j]$:

$$T_i[j] = \vec{U}_i \cdot \vec{x}[j] \qquad \begin{array}{l} i = 1, \dots n \\ j = 1, \dots p \end{array}$$

or $$\bar{\bar{T}} = \bar{\bar{U}}^* \cdot \bar{\bar{X}} = \bar{\bar{\Sigma}} \cdot \bar{\bar{W}}^*$$

with $$\bar{\bar{T}} = (\vec{T}[1], \vec{T}[2], \dots \vec{T}[p])$$

Each principal component $T_i[j]$ explains/captures a portion C_i of the total variance[1] $\sum_{k=1}^{p} C_k$ in the data.

Typically, retaining only the PCs with largest C_i captures most of the variance.

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(1) $\text{var}(\vec{x}) = \text{Trace}(\text{cov}(\vec{x})) = \text{Trace}(\bar{\bar{C}}) = \sum_{k=1}^{p} C_k$

APPENDIX :

Solution for inhomogeneous LTI ODEs :

$$\frac{d\vec{u}}{dt} = \bar{\bar{A}} \cdot \vec{u} + \vec{f} \qquad \text{with} \qquad \vec{u}(0) = \vec{u}_0$$

DRIVING FORCE

I.C.

by :

1) Variation of coefficients in the eigenmode expansion

2) Laplace and the eigen decomposition of $\bar{\bar{A}}$

INHOMOGENEOUS LTI ODEs :

$$\frac{d\vec{u}}{dt} = \bar{\bar{A}} \cdot \vec{u} + \underbrace{\vec{f}}_{\substack{\text{DRIVING} \\ \text{FORCE} \\ \text{(SOURCE)}}} \quad \text{with} \quad \underbrace{\vec{u}(0) = \vec{u}_0}_{\text{I.C.}}$$

- Solution by variation of coefficients in the eigenmode expansion:

Let $\vec{u}(t) = \sum_{i=1}^{N} \underbrace{c_i(t)}_{\substack{\text{COEFFICIENTS ARE} \\ \text{FUNCTION OF TIME}}} \vec{u}_i(t)$ with $\frac{d\vec{u}_i}{dt} = \bar{\bar{A}} \cdot \vec{u}_i = \lambda_i \cdot \vec{u}_i$

$$\Rightarrow \frac{d\vec{u}}{dt} = \sum_{i=1}^{N} \frac{dc_i}{dt} \cdot \vec{u}_i + \cancel{\sum_{i=1}^{N} c_i \frac{d\vec{u}_i}{dt}}$$

$$= \cancel{\sum_{i=1}^{N} c_i(t) \cdot \lambda_i \vec{u}_i} + \vec{f}$$

Let $\vec{f}(t) = \sum_{i=1}^{N} f_i(t) \vec{U}_i$ decomposition of $\vec{f}$ in basis $\{\vec{U}_i\}$

Also $\vec{u}_i = \vec{U}_i \, e^{\lambda_i t}$

$$\Rightarrow \quad \frac{dc_i}{dt} \cdot e^{\lambda_i t} = f_i(t) \qquad i = 1, \dots N$$

$$dc_i = f_i(t)\, e^{-\lambda_i t}\, dt$$

$$c_i(t) = c_i(0) + \int_0^t f_i(\vartheta)\, e^{-\lambda_i \vartheta}\, d\vartheta$$

$$\Rightarrow \vec{u}(t) = \sum_{i=1}^{N} c_i(t)\, \vec{u}_i(t) = \sum_{i=1}^{N} c_i(t)\, \vec{U}_i\, e^{\lambda_i t}$$

$$= \underbrace{\sum_{i=1}^{N} c_i(0)\, \vec{U}_i\, e^{\lambda_i t}}_{\text{I.C. ALONG EIGENMODES}} + \sum_{i=1}^{N} \int_0^t \underbrace{f_i(\vartheta)}_{\text{DRIVING FORCE}}\, \vec{U}_i\, e^{\lambda_i (t-\vartheta)}\, d\vartheta$$

CONVOLVED ALONG EIGENMODES

where $\vec{u}_0 = \sum_{i=1}^{N} c_i(0)\, \vec{U}_i$ I.C. DECOMPOSITION

$\vec{f}(t) = \sum_{i=1}^{N} f_i(t)\, \vec{U}_i$ DRIVING FORCE DECOMPOSITION

SPECIAL CASE

$\bar{\bar{A}}$ = SYMMETRIC :

($\vec{U}_i$ ORTHONORMAL)

$$c_i(0) = \vec{u}_0 \cdot \vec{U}_i$$

$$f_i(t) = \vec{f}(t) \cdot \vec{U}_i$$

$$\frac{d\vec{u}}{dt} = \bar{\bar{A}} \cdot \vec{u} + \vec{f} \qquad \text{with} \qquad \vec{u}(0) = \vec{u}_0$$

DRIVING FORCE (SOURCE)

I.C.

- Solution by LAPLACE and eigen decomposition of $\bar{\bar{A}}$:

$$\vec{u}(t) \xrightarrow{\text{Laplace}} \vec{U}(s)$$

$$s\,\vec{U}(s) - \vec{u}_0 = \bar{\bar{A}} \cdot \vec{U}(s) + \vec{F}(s)$$

$$s\,\vec{U}(s) - \bar{\bar{A}} \cdot \vec{U}(s) = \underbrace{\vec{u}_0}_{\text{I.C.}} + \underbrace{\vec{F}(s)}_{\text{DRIVING SOURCE}}$$

(NOTE: I.C. are equivalent to a driving source as a Dirac delta pulse at $t=0$!)

Eigen decomposition of $\bar{\bar{A}}$:

$$\bar{\bar{A}} = \bar{\bar{U}} \cdot \bar{\bar{\Lambda}} \cdot \bar{\bar{U}}^{-1}$$

where: $\bar{\bar{U}}$ is square with columns $\vec{U}_i$ eigenvectors

$\bar{\bar{\Lambda}}$ is diagonal with elements λ_i eigenvalues

$\bar{\bar{U}}^{-1}$ is the inverse of $\bar{\bar{U}}$ ($= \bar{\bar{U}}^T$ when $\bar{\bar{A}}$ = symmetric)

Corresponding EIGENMODE decomposition of $\vec{u}(s)$:

$$\vec{u}(s) = \bar{\bar{U}} \cdot \vec{\nu}(s)$$

Also:

$$\vec{u}_0 = \bar{\bar{U}} \cdot \vec{\nu}_0 \quad \text{decomposition of I.C.} \quad \left(\vec{\nu}_0 = \bar{\bar{U}}^{-1} \vec{u}_0 \right)$$

$$\vec{F}(s) = \bar{\bar{U}} \cdot \vec{\psi}(s) \quad \text{decomposition of SOURCE} \quad \left(\vec{\psi}(s) = \bar{\bar{U}}^{-1} \cdot \vec{F}(s) \right)$$

$$\Rightarrow s \cancel{\bar{\bar{U}}} \cdot \vec{\nu}(s) - \cancel{\bar{\bar{U}}} \bar{\bar{\Lambda}} \cancel{\bar{\bar{U}}^{-1}} \cancel{\bar{\bar{U}}} \vec{\nu}(s) = \cancel{\bar{\bar{U}}} \cdot \vec{\nu}_0 + \cancel{\bar{\bar{U}}} \cdot \vec{\psi}(s)$$

$$\left(s - \bar{\bar{\Lambda}} \right) \cdot \vec{\nu}(s) = \vec{\nu}_0 + \vec{\psi}(s)$$

Individual components:

$$(s - \lambda_i) \nu_i(s) = \nu_{0i} + \psi_i(s)$$

$$\nu_i(s) = \frac{\nu_{0i}}{s - \lambda_i} + \frac{1}{s - \lambda_i} \cdot \psi_i(s)$$

$$\Rightarrow \vec{u}(s) = \bar{\bar{U}} \cdot \vec{\nu}(s) = \sum_{i=1}^{N} \nu_i(s) \cdot \vec{u}_i$$

$$= \sum_{i=1}^{N} \frac{\nu_{0i}}{s - \lambda_i} \cdot \vec{u}_i + \sum_{i=1}^{N} \frac{1}{s - \lambda_i} \psi_i(s) \vec{u}_i$$

Inverse Laplace:

$$\vec{u}(t) = \sum_{i=1}^{N} \nu_{oi}\, e^{\lambda_i t}\, \vec{U}_i + \sum_{i=1}^{N} \int_0^t f_i(\vartheta)\, e^{\lambda_i(t-\vartheta)} d\vartheta\, \vec{U}_i$$

where $\psi_i(s) \xrightarrow{\text{inverse Laplace}} f_i(t)$, or

$$\vec{f}(t) = \sum_{i=1}^{N} f_i(t)\, \vec{U}_i \qquad \text{DRIVING SOURCE DECOMPOSITION}$$

Also, I.C. $\vec{u}(0) = u_0$, or

$$\vec{u}_0 = \sum_{i=1}^{N} \underbrace{\nu_{oi}}_{= c_i(0)} \vec{U}_i \qquad \text{I.C. DECOMPOSITION}$$

Same as solution by variation of coefficients!