FUNDAMENTAL CONCEPTS AND METHODS FOR SYSTEMS MODELING:

A Mathematical Foundation for the Description of Physical, Chemical, and Biological Processes

Outline of Lecture Unit 3

INTRODUCTORY CONCEPTS FROM THE SPECTRAL THEORY OF LINEAR OPERATORS

prepared by
Panos G. Georgopoulos
Computational Chemodynamics Laboratory
Department of Environmental and Community Medicine, UMDNJ-RWJMS
Departments of Chemical and Biochemical Engineering and Environmental Sciences, Rutgers

EOHSI, the Environmental and Occupational Health Sciences Institute
a joint institute of UMDNJ-R.W. Johnson Medical School and Rutgers, The State University of NJ
170 Frelinghuysen Road, Piscataway, NJ 08854

SOME CONCEPTS FROM THE SPECTRAL THEORY OF LINEAR OPERATORS

1 INTRODUCTION

1.1 Motivation for Study

Spectra and spectral representations (i.e. expressions in terms of eigenvalues and eigenvectors) of linear operators are useful in a wide variety of applications, including:

- Study of the existence of solutions of various types of linear equations.
- Study of the stability of linear differential and difference equations.
- Systematic construction of solutions of various types of linear equations (and, indirectly, of some nonlinear ones).
- Simplification of various types of mathematical models using the fact that eigenvectors are a most convenient set of basis vectors.
- Formulation and solution of various types of optimization problems.
- Formulation and solution of various types of approximation problems.

2 EIGENVALUES AND EIGENVECTORS: BASIC DEFINITIONS

Let $\boldsymbol{A}$ be a linear transformation on a linear vector space $\mathcal{V}$ (typically a Hilbert space $\mathcal{H}$).
The number λ_i is an *eigenvalue* and the vector $\mathbf{v}_i$ an *eigenvector* if

$$\boldsymbol{A}\mathbf{v}_i = \lambda_i \mathbf{v}_i, \quad \mathbf{v}_i \neq \mathbf{0}$$

or, equivalently

$$(\boldsymbol{A} - \lambda_i \boldsymbol{I})\, \mathbf{v}_i = \mathbf{0}, \quad \mathbf{v}_i \neq \mathbf{0}$$

So, eigenvectors span one-dimensional *invariant subspaces* of $\mathcal{V}$

- The set of eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is called the *spectrum* of $\boldsymbol{A}$
- The (invariant) subspace spanned by the eigenvector $\mathbf{v}_i$ corresponding to the eigenvalue λ_i is called the *eigenspace* of λ_i, $\mathcal{H}_{\lambda_i} = \{\mathbf{v}_i \in \mathcal{H} : \boldsymbol{A}\mathbf{v}_i = \lambda_i \mathbf{v}_i\}$

- Alternatively, the eigenspace of λ_i can be characterized as the null space of the linear transformation $(\boldsymbol{A} - \lambda_i \boldsymbol{I})$, usually denoted as $\mathcal{N}_i$.

If the linear transformation $\boldsymbol{A}$ on an n-dimensional space has a complete set of n linearly dependent eigenvectors, then it is called a *simple* transformation.

Note: While eigenvalues are uniquely defined, any scalar multiple $\alpha \mathbf{v}_i$ of $\mathbf{v} - i$ is also an eigenvector. This allows normalization: $\| \mathbf{v}_i \| = 1$

3 EIGENVALUES AND EIGENVECTORS: CALCULATION METHODS

3.1 Preliminaries

3.1.1 Some Types of Linear Operators (... i.e. more semantics)

A linear operator $\boldsymbol{A}$ on a linear vector space with inner product $(\mathbf{x} \cdot \mathbf{y})$ is called

1. the *adjoint* $\hat{\boldsymbol{B}}$ of operator $\boldsymbol{B}$ if $\forall \mathbf{x}, \mathbf{y}$

$$(\mathbf{x} \cdot \boldsymbol{A}\mathbf{y}) = (\boldsymbol{B}\mathbf{x} \cdot \mathbf{y})$$

   - The matrix of the adjoint of an operator with matrix $\mathbf{A}$ is $\overline{\mathbf{A}}^{\top}$, i.e. the transpose complex conjugate of $\mathbf{A}$.

2. a *unitary,* $\boldsymbol{U}$, operator if it preserves lengths and angle.
   - The adjoint of an unitary operator is the inverse of the operator.
   - The columns of the matrix representation of a unitary operator form an orthonormal basis.

3. a *self-adjoint* or *Hermitian* operator if

$$(\mathbf{x} \cdot \boldsymbol{H}\mathbf{y}) = (\boldsymbol{H}\mathbf{x} \cdot \mathbf{y})$$

4. a *normal,* $\boldsymbol{N}$, operator, if it commutes with its adjoint, i.e. if

$$\hat{\boldsymbol{N}}\boldsymbol{N}\mathbf{x} = \boldsymbol{N}\hat{\boldsymbol{N}}\mathbf{x}$$

3.1.2 Determinants of Linear Operators

The determinant $\det(\boldsymbol{A})$ of the linear transformation $\boldsymbol{A}$ on $\mathcal{V}$ is a map to the associated scalar field that is defined through the following relations:

- $\boldsymbol{A}\mathbf{x} = \mathbf{0}$ has a non-zero solution iff $\det(\boldsymbol{A}) = 0$
- If $\boldsymbol{K}$ and $\boldsymbol{L}$ are linear operators, then $\det(\boldsymbol{L}\boldsymbol{K}) = \det(\boldsymbol{L}) \det(\boldsymbol{K})$
- $\det(\boldsymbol{I}) = 1$
- $\det(\boldsymbol{A}) = \det\left(\boldsymbol{A}^{\top}\right)$

It is obvious (from the way we just introduced it) that $\det(\boldsymbol{A})$ is *not* associated with the particular matrix representation $\mathbf{A}$ of the linear operator (although the matrix is typically used to calculate the determinant according to the known rules and techniques of elementary linear algebra). Therefore it must be the same for all such representations.

3.2 Determination of Eigenvalues

For finite dimensional linear transformations on $\mathcal{E}_n$, $(\boldsymbol{A}-\lambda_i\boldsymbol{I})\,\mathbf{v}_i=\mathbf{0}$ is represented by the corresponding matrix equation $(\mathbf{A}-\lambda_i\mathbf{I})\,\mathbf{v}_i=\mathbf{0}$ (set of n homogeneous equations). The requirement for the existence of nontrivial solutions is

$$\operatorname{rank}(\mathbf{A}-\lambda_i\mathbf{I})<n \Leftrightarrow \det(\mathbf{A}-\lambda_i\mathbf{I})=0$$

i.e.

$$\boldsymbol{\Delta}(\lambda)=\det(\mathbf{A}-\lambda_i\mathbf{I})=(-\lambda)^n+c_{n-1}\lambda^{n-1}+c_{n-2}\lambda^{n-2}+\ldots+c_1\lambda+c_0=0\Rightarrow$$
$$\Rightarrow\boldsymbol{\Delta}(\lambda)=(\lambda)(-1)^n(\lambda-\lambda_1)(\lambda-\lambda_2)\ldots(\lambda-\lambda_n)=0$$

where $\boldsymbol{\Delta}(\lambda)$ is the *characteristic polynomial* of the linear operator or *any* of its matrix representations.
If the *algebraic multiplicity* of λ_i is m_i, then

$$\boldsymbol{\Delta}(\lambda)=(\lambda)(-1)^n(\lambda-\lambda_1)^{m_1}(\lambda-\lambda_2)^{m_2}\ldots(\lambda-\lambda_n)^{m-n}$$

where $m_1+m_2+\ldots+m_n=n$.
So, determining eigenvalues for $\boldsymbol{A}$ is equivalent to factoring an nth degree polynomial. In practice, iterative methods are used for constructing eigenvalues and eigenvectors.

Note: useful relationships between $\mathbf{A}$, c_i and λ_i:

1. if c_i are real and λ_i is a complex eigenvalue, then so is $\overline{\lambda}_i$
2. $\operatorname{tr}(\mathbf{A})=\lambda_1+\lambda_2\ldots+\lambda_n=(-1)^{n+1}c_{n-1}$
3. $\det(\mathbf{A})=\lambda_1\lambda_2\ldots\lambda_n=c_0$

3.3 Determination of Eigenvectors

3.3.1 Case of Distinct Eigenvalues ($m_i=1$ for all i)

In this case there exist n linearly independent eigenvectors. Also, $\operatorname{rank}(\mathbf{A}-\lambda_i\mathbf{I})=n-1$ and a nontrivial solution to $(\mathbf{A}-\lambda_i\mathbf{I})\,\mathbf{v}_i=\mathbf{0}$ is given by any nonzero column of the matrix of *cofactors* (or *signed minors*) of $(\mathbf{A}-\lambda_i\mathbf{I})$.
In practice the $n\times n$ *modal matrix* $\mathbf{M}=[\mathbf{v}_1\,\mathbf{v}_2\ldots\mathbf{v}_n]$ is calculated from the equation

$$\mathbf{AM}=\mathbf{M\Lambda},\quad \mathbf{\Lambda}=\operatorname{diag}[\lambda_1,\lambda_2,\ldots,\lambda_n]$$

Since the eigenvectors are l.i., $\operatorname{rank}(MM)=n$, so its inverse exists and

$$\mathbf{\Lambda}=\mathbf{M}^{-1}\mathbf{AM}$$

This is called a *similarity transformation.* A square matrix with distinct eigenvalues can always be diagonalized by a similarity transformation.
When $\mathbf{M}^{-1}=\mathbf{M}^{\top}$, $\mathbf{A}$ can be diagonalized by the *orthogonal transformation* $\mathbf{\Lambda}=\mathbf{M}^{\top}\mathbf{AM}$.

3.3.2 Case of Multiple Eigenvalues ($m_i > 1$ for some i)

The number of linearly independent eigenvectors associated with a given λ_i of algebraic multiplicity m_i is equal to $q_i = n - \mathrm{rank}(\mathbf{A} - \lambda_i \mathbf{I}), \quad 1 \le q_i \le m_i$. This number is also called the *degeneracy* of $(\mathbf{A} - \lambda_i \mathbf{I})$ or the *geometric multiplicity* of λ_i, i.e. the dimension of the space spanned by its eigenvectors.

- When $q_i = m_i$ (full degeneracy) there is a full set of m_i eigenvectors associated with λ_i (the case of distinct eigenvalues is a special case of this, foe $m_i = 1$).
- When $q_1 = 1$ (simple degeneracy) there is only one eigenvector associated with λ_i. An additional set of $m_i - 1$ vectors, the *generalized eigenvectors,* or *companion vectors* of the associated eigenvector can be found for λ_i and so n linearly independent vectors (eigenvectors or generalized eigenvectors) can be found for $\mathbf{A}$. In this case it is not possible to diagonalize $\mathbf{A}$ by a similarity transformation; however, using a modal matrix $\mathbf{M}$ that contains the the eigenvectors and the generalized eigenvectors, a *Jordan block* matrix $\mathbf{J}$ can be constructed:

$$\mathbf{J} = \mathbf{M}^{-1}\mathbf{A}\mathbf{M}, \quad \mathbf{J} = [\mathbf{J}_1, \mathbf{J}_2, \dots \mathbf{J}_n], \quad \mathbf{J}_i = \begin{bmatrix} \lambda_i & 1 & & & \\ & \lambda_i & 1 & & \\ & & & \ddots & \\ & & & & 1 \\ & & & & \lambda_i \end{bmatrix}$$

- In the general case $1 \le q_i \le m_i$ there will be q_i eigenvectors (and corresponding Jordan blocks) and $m_i - q_i$ generalized eigenvectors associated with λ_i. However, since there are more than one eigenvectors for each λ_i there is some ambiguity as to which eigenvector are the generalized eigenvectors associated with; iterative methods for determining generalized eigenvectors are a major subject of numerical linear algebra. The transformation $\mathbf{M}^{-1}\mathbf{A}\mathbf{M}$ again gives a Jordan block matrix.

3.4 Spectral Properties of Some Special Types of Operators

1. The characteristic polynomial of the adjoint of an operator is the complex conjugate of the characteristic polynomial of the original operator.
2. The eigenvalues of Hermitian operators are real and eigenvectors corresponding to distinct eigenvalues are orthogonal.
3. A normal operator and its adjoint have the same eigenvectors and eigenvectors corresponding to distinct eigenvalues are orthogonal.

4 SPECTRAL DECOMPOSITION AND INVARIANCE PROPERTIES

4.1 Preliminaries

4.1.1 Sums and Direct Sums of Vector Spaces

A linear vector space $\mathcal{X}$ is the sum of the linear vector spaces $\mathcal{U}$ and $\mathcal{V}$, $\mathcal{X} = \mathcal{U} + \mathcal{V}$, if

$$\forall \mathbf{x} \in \mathcal{X} : \mathbf{x} = \mathbf{u} + \mathbf{v}, \ \mathbf{u} \in \mathcal{U}, \ \mathbf{v} \in \mathcal{V}$$

If there is one and only one pair $\mathbf{u}, \mathbf{v}$ for each $\mathbf{x}$, then $\mathbf{x}$ is called the *direct sum* of $\mathcal{U}$ and $\mathcal{V}$,

$$\mathcal{X} = \mathcal{U} \oplus \mathcal{V}$$

and the only vector common in both $\mathcal{U}$ and $\mathcal{V}$ is $\mathbf{0}$. In this case

$$\dim(\mathcal{X}) = \dim(\mathcal{U}) + \dim(\mathcal{V})$$

Example

1. Consider the subspace $\mathcal{U}$ of $\mathcal{X}$ and its orthogonal complement $\mathcal{U}^{\perp}$.
   Then, $\mathcal{X} = \mathcal{U} \oplus \mathcal{U}^{\perp}$ and $\dim(\mathcal{X}) = n, \dim(\mathcal{U}) = m \Rightarrow \dim\left(\mathcal{U}^{\perp}\right) = n - m$.
   Furthermore, if $\mathbf{x} = \mathbf{u} + \mathbf{v}, \mathbf{x} \in \mathcal{X}, \mathbf{u} \in \mathcal{U}, \mathbf{v} \in \mathcal{U}^{\perp}$, then $\| \mathbf{x} \|^2 = \| \mathbf{u} \|^2 + \| \mathbf{v} \|^2$.

4.1.2 Reciprocal Bases of Linear Vector Spaces

Let $\{\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n\}$ be a base of $\mathcal{E}_n$ and $\mathbf{F} = [\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n]$ (an $n \times n$ matrix). The set of vectors $\{\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_n\}$, where $\mathbf{g}_i$ is defined as the (conjugate) transpose of the i-th *row* of $\mathbf{F}^{-1}$, is called the *reciprocal basis* of $\{\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n\}$. The following relation is then satisfied: $\mathbf{f}_i \mathbf{g}_j = \delta_{ij}$.
Furthermore, if the expansion of $\mathbf{x} \in \mathcal{E}_n$ is $\sum_{i=1}^{n} x_i \mathbf{f}_i$, the components of $\mathbf{x}$ can be expressed in terms of the reciprocal base vectors as

$$x_i = (\mathbf{g}_i \cdot \mathbf{x}) \Rightarrow \mathbf{x} = \sum_{i=1}^{n} ((\mathbf{g}_i \cdot \mathbf{x}))\, \mathbf{f}_i$$

4.1.3 Dimension of Eigenspaces

With $\boldsymbol{A}$ defined on $\mathcal{X}$, $\mathcal{N}_i$ is an invariant subspace of $\mathcal{X}$ under $\boldsymbol{A}$ and

$$\dim(\mathcal{N}_i) = q_i = n - \operatorname{rank}(\boldsymbol{A} - \lambda_i \boldsymbol{I})$$

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4.2 Decomposition of a Vector Space by an Operator

If $\boldsymbol{A}$ on an n-dimensional $\mathcal{X}$ is simple with p distinct eigenvalues (i.e. it either has $p = n$ distinct eigenvalues or, if $p < n$, the repeated eigenvalues have full degeneracy and therefore there are still n linearly independent eigenvectors), then

$$\mathcal{X} = \mathcal{N}_1 \oplus \mathcal{N}_2 \oplus \ldots \mathcal{N}_p$$

Note: If $\boldsymbol{A}$ is normal, $\mathcal{N}_i, \mathcal{N}_j$ are orthogonal to each other $\forall i \neq j$. Normal transformations are a subset of simple transformations.

4.3 Spectral Representation of a Linear Operator

If $\boldsymbol{A}$ is a simple linear transformation on the n-dimensional space $\mathcal{X}$, its eigenvectors $\{\mathbf{v}_i\}$ form a basis for $\mathcal{X}$. If $\{\mathbf{u}_i\}$ are the reciprocal basis vectors for $\{\mathbf{v} - i\}$, then every $\mathbf{x} \in \mathcal{X}$ can be written as

$$\mathbf{x} = \sum_{i=1}^{n} (\mathbf{u}_i \cdot \mathbf{x})\ \mathbf{v}_i$$

and therefore

$$\boldsymbol{A}\mathbf{x} = \sum_{i=1}^{n} (\mathbf{u}_i \cdot \mathbf{x})\ \boldsymbol{A}\mathbf{v}_i = \sum_{i=1}^{n} \lambda_i\ (\mathbf{u}_i \cdot \mathbf{x})\ \mathbf{v}_i$$

This is a *spectral representation*[1] of $\boldsymbol{A}$.
If $\boldsymbol{A}$ is normal, then its eigenvectors are mutually orthogonal and the reciprocal basis vectors can be made equal to the eigenvectors through normalization; more simply in the orthonormal basis the components of $\mathbf{x}$ are given by the inner product of $\mathbf{x}$ and the basis vectors:

$$\mathbf{x} = \sum_{i=1}^{n} (\mathbf{v}_i \cdot \mathbf{x})\ \mathbf{v}_i$$

and therefore

$$\boldsymbol{A}\mathbf{x} = \sum_{i=1}^{n} \lambda_i\ (\mathbf{v}_i \cdot \mathbf{x})\ \mathbf{v}_i$$

This is a most convenient way for representing linear operators.

5 A PREVIEW OF APPLICATIONS: THE SOLUTION OF LINEAR ODE SYSTEMS

A linear differential operator of arbitrary order can be set in matrix form, as a finite system of first order ode's:

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{A}\mathbf{x} = \mathbf{A}\mathbf{x}$$

This equation is governs a wide variety of linear "lumped parameter" or "finite-dimensional" models of process systems.
A most important theorem of mathematics states that:
(a) The differential equation $\frac{d\mathbf{x}}{dt} = \boldsymbol{A}\mathbf{x}$ always has a nontrivial solution when $\det(\boldsymbol{A}) \neq 0$, and
(b) The initial value problem $\frac{d\mathbf{x}}{dt} = \boldsymbol{A}\mathbf{x}, \mathbf{x}(t_0) = \mathbf{x}_0$ has one and only one solution.
Furthermore, the set of solutions of $\frac{d\mathbf{x}}{dt} = \boldsymbol{A}\mathbf{x}$ is a linear vector space.

Considet the case where $\mathbf{A}$ is an $n \times n$ matrix. The vector function $\mathbf{x}(t) = \exp(\lambda t)\mathbf{v}$ is a solution of $\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x}$ if and only if λ is an eigenvalue of $\mathbf{A}$ and $\mathbf{v}$ is an eigenvector associated with λ. Indeed, $\mathbf{x}(t) = \exp(\lambda t)\mathbf{v}$ would be a solution of $\frac{dx}{dt} = \mathbf{A}\mathbf{x}$ if and only if $\lambda \exp(\lambda t)\mathbf{v} = \exp(\lambda t)\mathbf{A}\mathbf{v}$. Since $\exp(\lambda t)$ is never zero the result $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ is obtained directly.
Each eigenvalue λ determines an infinite number of solutions of the form $\mathbf{x}(t) = \exp(\lambda t)\mathbf{v}$; the number of independent solutions depends on the number of independent eigenvectors associated with λ. If there are n independent eigenvectors $\{\mathbf{v}_i\}$, then

$$\mathbf{x}_1(t) = e^{\lambda_1 t}\mathbf{v}_1, \mathbf{x}_2(t) = e^{\lambda_2 t}\mathbf{v}_2, \ldots, \mathbf{x}_n(t) = e^{\lambda_n t}\mathbf{v}_n$$

form a basis for the solution space of $\frac{d\mathbf{x}}{dt} = \boldsymbol{A}\mathbf{x}$ and therefore the general form of the solution is

$$\mathbf{x}(t) = c_1\, e^{\lambda_1 t}\mathbf{v}_1 + c_2\, \mathbf{x}_2(t) = e^{\lambda_2 t}\mathbf{v}_2 + \ldots + c_n\mathbf{x}_n(t)\ e^{\lambda_n t}\mathbf{v}_n$$

More on this appoach - in Lecture Unit 4.

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[1] At a later time we will see how this expression is usually set in dyadic form.

6 PROBLEMS FOR THE MATERIAL OF LECTURE UNIT 3

A problem set covering material of this lecture unit will be given with the outline of Lecture Unit 4. (This is when problem set # 2 is also due). For practice, however, review (once again!) the fundamentals of algebraic equation systems and (using any linear algebra book) try to find simple examples for the various types of operators (i.e. self-adjoint, unitary, normal) that are mentioned in this outline. Also, prove that the matrices of adjoint, Hermitian and unitary operators have the properties listed in 3.1.1 and 3.4.