2. Lectures 3,4:

Topics for these lectures:

- ◇ Solvability conditions for linear systems
- ◇ Eigenvalues and eigenvectors with applications to:
  - – Solution of linear systems of ODE
  - – Oscillators
  - – Iterative solution of linear systems
- ◇ Introduction to SVD

2.1. **Solvability conditions for linear systems.** Let A be $n \times n$ and consider $Ax = b$. If A is not singular, then this system has a unique solution $x = A^{-1}b$. Can it have a solution if A is singular? The answer depends on the relationship between A and b.

Recall, that Ax is always a combination of columns of A, no matter what x is. Therefore, for $Ax = b$ to have a solution, b must be a combination of columns of A. In other words, b must be in the column space of A, $b \in C(A)$. This condition on b can be expressed as an orthogonality condition, as any vector in $C(A)$ must be orthogonal to the left nullspace of A, $N\left(A^T\right)$

$$y^T b = 0, \qquad \text{solvability condition for } Ax = b, \text{ where } A^T y = 0.$$

The equation $A^T y = 0$ is called the adjoint problem.

Example 9. For example, matrix

$$A = \begin{bmatrix} 1 & 0 & 2 \\ 1 & 2 & 8 \\ 0 & -1 & -3 \end{bmatrix}$$

is singular because $A(:,3) = 2A(:,1)+3A(:,2)$. Its left nullspace is spanned by $y = \begin{bmatrix} 1 & -1 & -2 \end{bmatrix}$, since $1 \cdot row_1 - row_2 - 2 \cdot row_3 = 0$, or:

$$A^T y = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 2 & -1 \\ 2 & 8 & -3 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \\ -2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Therefore, $Ax = b$ will have a solution only if b satisfies $y^T b = b_1 - b_2 - 2b_3 = 0$. In fact, if that condition is satisfied, $Ax = b$ will have infinitely many solutions, as one can add to x the nullspace of A, $Ax_0 = 0$, so that if x is a solution then $x+x_0$ is also a solution, $A(x + x_0) = Ax+Ax_0 = b$. This is the Fredholm alternative.

2.2. **Eigenvalues and eigenvectors.** From the very definition $As_i = \lambda_i s_i$, we can deduce the factorization

$$AS = S\Lambda \tag{2.1}$$

where columns of S are eigenvectors s_i and Λ is a diagonal matrix with e-values λ_i on its diagonal. If we recall how the matrices multiply this factorization easily follows as a shorthand for

$$\begin{bmatrix} | & | & & | \\ As_1 & As_2 & \dots & As_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \lambda_1 s_1 & \lambda_2 s_2 & \dots & \lambda_n s_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ s_1 & s_2 & \dots & s_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & \cdots \\ 0 & \lambda_2 & 0 \\ \vdots & & \ddots \end{bmatrix}.$$

Then, if S is full rank, A can be decomposed as

$$A = S\Lambda S^{-1} \tag{2.2}$$

which is called the spectral decomposition. Not all matrices enjoy this kind of factorization, but an important class of symmetric matrices does. We will return to this later. For now we just assume that the factorization is possible and illustrate how it can be useful in various problems.

Another way of looking at this factorization follows from the fact that $Ax = b$ can be seen as a expressing the vector b in terms of columns of matrix A:

$$b = x_1 a_1 + x_2 a_2 + ... + x_n a_n.$$

In other words, if columns of A form a basis, this is simply a change of basis formula, expressing vector b in a new basis, rather than standard basis made of 1's and 0. And $x = A^{-1}b$ are the coordinates of b in that new basis. Indeed, b in the standard basis

$$e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \; e_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \dots$$

is

$$b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix} = b_1 e_1 + b_2 e_2 + \dots,$$

showing that b_i is the component of b in the direction of e_i. And so x_i is similarly a component of b, but now in the direction of a_i.

Then if we act with $A = S\Lambda S^{-1}$ on x, we get

$$Ax = S\Lambda \left(S^{-1}x\right).$$

This can be interpreted, reading from right to left, as saying that:

(1) change the basis to that of the eigenvectors to find new components of x in that basis as $S^{-1}x$;
(2) then stretch the new coordinates by eigenvalues: $\Lambda \left(S^{-1}x\right)$; and
(3) return to the original basis by multiplying with S.

2.2.1. *Solution of linear systems of ODE.* Suppose, we need to solve a system of linear differential equations of the form

$$\frac{du}{dt} = Au, \tag{2.3}$$

where A is an $n \times n$ constant matrix, u is an n-vector, and the initial condition is $u(0) = u_0$. For a scalar equation, the solution would be $u = u_0 e^{At}$. In fact, for the system, we can write almost the same solution

$$u = e^{At} u_0 \tag{2.4}$$

provided the exponential can be given some meaning. Here is where the spectral decomposition comes to help.

Let $A = S\Lambda S^{-1}$ in (2.3). Then

$$\begin{aligned} \frac{du}{dt} &= S\Lambda S^{-1}u = S\Lambda\left(S^{-1}u\right) \\ S^{-1}\frac{du}{dt} &= \Lambda\left(S^{-1}u\right) \\ v &= S^{-1}u \\ \frac{dv}{dt} &= \Lambda v. \end{aligned}$$

The last equation breaks into n scalar equations with simple solutions:

$$\frac{dv_i}{dt} = \lambda_i v_i, \qquad v_i = v_{i0}e^{\lambda_i t}.$$

The components v_i can be put in a vector as

$$v = \begin{bmatrix} e^{\lambda_1 t} & 0 & \cdots \\ 0 & e^{\lambda_2 t} & 0 \\ \vdots & & \ddots \end{bmatrix} \begin{bmatrix} v_{10} \\ v_{20} \\ \vdots \end{bmatrix} = e^{\Lambda t}v_0,$$

where $e^{\Lambda t}$ is *defined* to be the diagonal matrix here. Now we put things back to find the original unknown u:

$$u = Sv = Se^{\Lambda t}v_0 = Se^{\Lambda t}S^{-1}u_0.$$

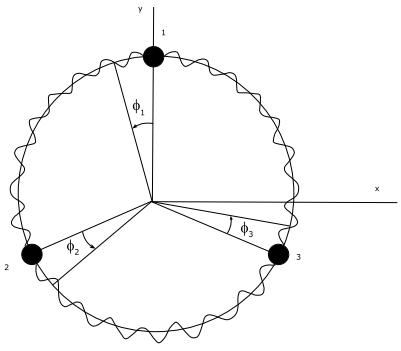
The matrix multiplying u_0 here is exactly what is meant by e^{At} in (2.4).

We can see the same in terms of the change of basis. In the basis of eigenvectors, the solution vector u will have components $v = S^{-1}u$. These components satisfy the differential equation

$$\frac{dv}{dt} = S^{-1}\frac{du}{dt} = S^{-1}Au = S^{-1}ASv = \Lambda v,$$

as before. That is, the calculation above and the magic decoupling of the system into n separate equations is a consequence of the change of the frame. The basis made of the eigenvectors of A is the best basis in which to solve the problem. In each eigenvector direction we have a clean single exponential with the growth rate given by the corresponding eigenvalue.

2.2.2. *Linear oscillators*



Consider oscillations of three beads of unit mass connected to each other on a ring with springs of unit spring constant. The equations of motion are derived simply using Newton's law as, for example, for mass 1:

$$m_1 r\ddot{\phi}_1 = k_{12}r\left(\phi_2 - \phi_1\right) + k_{13}r\left(\phi_3 - \phi_1\right)$$

with mass m_i, radius of the circle r and stiffness coefficients k_{ij} between bead i and j.

With the assumptions of unit everything, we get the system:

$$\begin{aligned} \ddot{\phi}_1 &= -2\phi_1 + \phi_2 + \phi_3, \\ \ddot{\phi}_2 &= \phi_1 - 2\phi_2 + \phi_3, \\ \ddot{\phi}_3 &= \phi_1 + \phi_2 - 2\phi_3, \end{aligned} \tag{2.5}$$

and in matrix form

$$\ddot{u} = Au, \tag{2.6}$$

where

$$u = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix}, \qquad A = \begin{bmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{bmatrix}.$$

One way to proceed is to look for a solution of the form (normal modes):

$$u = ve^{\omega t}, \tag{2.7}$$

where v is a constant vector and ω is a constant scalar, both of which are to be determined. Plug into (2.6), then:

$$Av = \omega^2 v,$$

which shows that v is the eigenvector of A corresponding to the eigenvalue $\lambda = \omega^2$. Therefore, once we find the eigenvectors and eigenvalues of A, then (2.7) would give us the desired solutions.

We do not have to look for a solution like above. We can start by changing the basis: $v = S^{-1}u$. This introduces new variables v_1, v_2, ... in the vector v which are good combinations of the original variables u_1, u_2,..., u_n. Then $\ddot{v} = S^{-1}\ddot{u} = S^{-1}ASv = \Lambda v$. Then solving this diagonal system we get $v_i(t) = a_i \cos(\lambda_i t) + a_i \sin(\lambda_i t)$. Then back to the original basis $u = Sv$.

Note that A is a symmetric matrix, therefore all of its eigenvalues must be real and its set of eigenvectors is complete (even if some of the eigenvalues are repeated) and can be chosen orthogonal. We will come back to the discussion of symmetry.

First, calculate the e-values:

$$|A - \lambda I| = \begin{vmatrix} -2-\lambda & 1 & 1 \\ 1 & -2-\lambda & 1 \\ 1 & 1 & -2-\lambda \end{vmatrix} = -\lambda(\lambda+3)^2 = 0,$$

Therefore, the eigenvalues are: $\lambda_1 = 0$, $\lambda_2 = \lambda_3 = -3$.

Next, e-vectors:

$$\lambda_1 = 0: \quad Av_1 = 0, \quad \begin{bmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{bmatrix} v_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \Rightarrow \quad v_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\lambda_2 = -3: \quad (A - \lambda_2 I)v_2 = 0, \quad \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} v_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \Rightarrow v_2 = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \text{ and } v_3 = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}.$$

Note that v_1, v_2, and v_3 are mutually orthogonal. We could have chosen

$$v_3^0 = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix},$$

but then it would not have been orthogonal to v_2. One can always orthogonalize such vectors by Gram-Schmidt procedure: faced with v_3^0, modify it as $v_3 = v_3^0 + cv_2$ by choosing the constant c so that $v_3^T v_2 = 0$. Then $0 = v_3^T v_2 = \left(v_3^0\right)^T v_2 + cv_2^T v_2$, from which $c = -\frac{\left(v_3^0\right)^T v_2}{v_2^T v_2} = -\frac{1}{2}$ so that

$$v_3 = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} \quad \text{or} \quad v_3 = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}.$$

Note here that

$$v_3 = v_3^0 - \frac{v_3^0 \cdot v_2}{v_2 \cdot v_2} v_2 = v_3^0 - v_2 \frac{v_2^T v_3^0}{v_2^T v_2} = \left(I - \frac{v_2 v_2^T}{v_2^T v_2}\right) v_3^0 = \left(I - P_2\right) v_3^0,$$

where P_2 is the projection matrix to the direction of v_2. That is, new v_3 is the old v_3 minus its part along the direction of v_2. That leaves the part of v_3 that is perpendicular to v_2. In fact, $I - P_2$ is the projection to the direction perpendicular to v_2.

The most general solution corresponding to $\lambda = 0$ is not just a constant vector v_1, but takes the form $u_1 = f(t) v_1$ with some function of time $f(t)$. Plug this into (2.6) to find that $\ddot{f} v_1 = f A v_1 = 0$, from which $\ddot{f} = 0$ and $f(t) = c_0 + c_1 t$. Note the analogy with a single equation $\ddot{x} + \omega^2 x = 0$, whose solutions are sines and cosines if $\omega \neq 0$, but $c_0 + c_1 t$ if $\omega = 0$.

Now once we have the e-values and e-vectors of A, the general solution is

$$u = (c_0 + c_1 t) v_1 + \left[c_2 \cos\left(\sqrt{3}t\right) + c_3 \sin\left(\sqrt{3}t\right)\right] v_2 + \left[c_4 \cos\left(\sqrt{3}t\right) + c_5 \sin\left(\sqrt{3}t\right)\right] v_3. \tag{2.8}$$

In order to better understand the meaning of the three separate components of u, let us now look for the solutions of the following initial-value problems.

(1) First, let

$$u(0) = 0, \quad \dot{u}(0) = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = v_1. \tag{2.9}$$

This initial condition means no initial displacements and equal initial velocities for all beads. Now we need to find the constants in (2.8):

$$u(0) = 0: \;\; c_0 v_1 + c_2 v_2 + c_4 v_3 = 0, \quad \dot{u}(0) = v_1: \;\; c_1 v_1 + \sqrt{3} c_3 v_2 + \sqrt{3} c_5 v_3 = v_1. \tag{2.10}$$

Since vectors v_1, v_2, and v_3 are orthogonal, (2.10) can hold only if $c_0 = c_2 = c_4 = 0$ (first equation) and $c_1 = 1, \quad c_3 = c_5 = 0$ (second equation). Finally,

$$u(t) = t \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \longleftarrow \text{ pure spinning motion.}$$

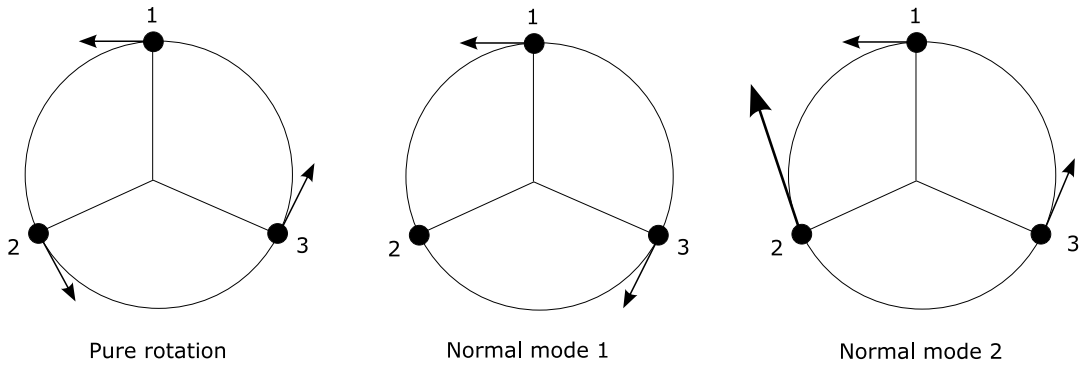


FIGURE 2.1. Three basic types of motion that superpose to give the general solution of the problem.

(2) Now let

$$u(0) = 0, \quad \dot{u}(0) = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} = v_2. \tag{2.11}$$

This initial condition means no initial displacements and equal but opposite initial velocities for masses 1 and 3 and no initial velocity for mass 2. Then $c_0 = c_2 = c_4 = 0$ again due to $u(0) = 0$ and $c_3 = 1/\sqrt{3}$, $c_1 = c_5 = 0$ due to $\dot{u}(0) = v_2$, so that the final solution is

$$u(t) = \frac{1}{\sqrt{3}} \sin\left(\sqrt{3}t\right) \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}.$$

This solution corresponds to masses 1 and 3 moving in opposite directions while the mass 2 stays at rest at all times (normal mode 1 in figure above). Mode 2 in the figure also shows the character of oscillations corresponding to the third e-vector, v_3. In this case

$$u(t) = \frac{1}{\sqrt{3}} \sin\left(\sqrt{3}t\right) \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

and masses 1 and 3 move together with the same amplitude, while mass 2 is in opposite phase and with amplitude twice as large as that of mass 1 or 3.

Thus, the solution to any initial-value problem for this system is a superposition of three elementary solutions: pure rotation, and the two normal modes. A side note: if one adds all three equations (2.5), then one finds that $\dot{\phi}_1 + \dot{\phi}_2 + \dot{\phi}_3 = constant$, which expresses the conservation of angular momentum.

2.2.3. *Iterative solution of linear systems.* Solution of large systems of linear equations are often found by iterative methods rather than direct methods such as elimination. The idea is to split the matrix A into two parts $A = A_1 + A_2$ such that solving for $A_1 x = b$ is easy, for example, because A_1 is diagonal. Then $Ax = b$ is rewritten as

$$A_1 x = b - A_2 x$$

which is then used to do iterations. Starting with some initial value $x = x_0$, we iterate

$$A_1 x_{k+1} = b - A_2 x_k$$

hoping that these iterations will converge to the solution, in which case x_{k+1} will be very close to x_k. Since $x_{k+1} = A_1^{-1} b - A_1^{-1} A_2 x_k$, then convergence of such iterations depends on the e-values of $B = A_1^{-1} A_2$. Indeed, if x is the exact solution, then subtracting previous two displayed equations, we get

$$\begin{aligned} A_1 (x_{k+1} - x) &= -A_2 (x_k - x), \\ x_{k+1} - x &= -A_1^{-1} A_2 (x_k - x), \\ e_{k+1} &= -B e_k, \end{aligned}$$

where e_k denotes the error at iteration k. Suppose B has e-values λ_i with corresponding e-vectors s_i: $Bs_i = \lambda_i s_i$. Then, if $e_0 = \sum_{i=1}^n a_i s_i$, we find that $e_k = -\sum_{i=1}^n a_i \lambda_i^k s_i$ which converges only if all $|\lambda_i| < 1$. To have fast convergence, one needs to split A such that the largest e-value of B is as small as possible.

Depending on how the splitting is done, we get several versions of the method. Two classical methods are Jacobi and Gauss-Seidel.

Example. Jacobi iterations. Here $A = D + L + U$ with $D = diag(A)$ and U, L upper and lower parts of A. Then take $A_1 = D$, $A_2 = U + L = A - D$. The iterations are very simple then.

Example. Gauss-Seidel iterations. Now instead of taking $A_1 = D$, we take $A_1 = D + L$, the whole lower part of A (*tril(A) in Matlab*). Then we get a triangular system to solve, which is also easy.

Example 10. Consider a linear system $Ax = b$ with

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & -2 \\ 0 & -1 & 2 \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

The exact solution is $x = \begin{bmatrix} -5 & 7 & 4 \end{bmatrix}^T$. Both Jacobi and Gauss-Seidel converge with $x_0 = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T$, even though it takes 257 iterations for Jacobi to reach $tol = 10^{-6}$, while it takes 120 for Gauss-Seidel.

If we switch the first two rows of A, then both methods fail to converge because then the matrix B will have eigenvalues larger than 1 in magnitude.

```
%% Iterative solution of linear systems
% will use Jacobi and Gauss-Seidel to solve Ax=b with A=A1+A2
% convergence of the iterations will depend on the eigenvalues of
% B = inv(A1)*A2 = A1\A2:
% for convergence, eigenvalues of B must be <1 in magnitude
clear all;

A = [2 1 1; 1 2 -2; 0 -1 2] %will converge
%A = [1 2 -2; 2 1 1; 0 -1 2] %will not converge
if rank(A)<3, disp('singular matrix'), return, end
b = [1 1 1]';
x_exact = A\b

tol = 10^-6; %error tolerance for convergence
x = [1 1 1]'; %initial guess
err = 1; count = 0;

solver = 'gs'; % 'jac' or 'gs'
switch solver
case 'jac' %Jacobi
    A1 = diag(diag(A));
    A2 = A - A1;
    B = A1\A2;
    while err > tol
        x = A1\(b - A2*x);
        err = norm(x-x_exact);
        if err > 100, break, end
        count = count +1;
    end
    disp (['iterations ',num2str(count),', err = ',num2str(err)])

case 'gs' % Gauss-Seidel
    A1 = tril(A); %lower triangular part of A including diagonal
    A2 = A - A1;
    B = A1\A2;
    while err > tol
        x = A1\(b - A2*x);
        err = norm(x-x_exact);
        if err > 100, break, end
        count = count +1;
    end
    disp (['iterations ',num2str(count),', err = ',num2str(err)])

    otherwise
    disp 'another case'
end
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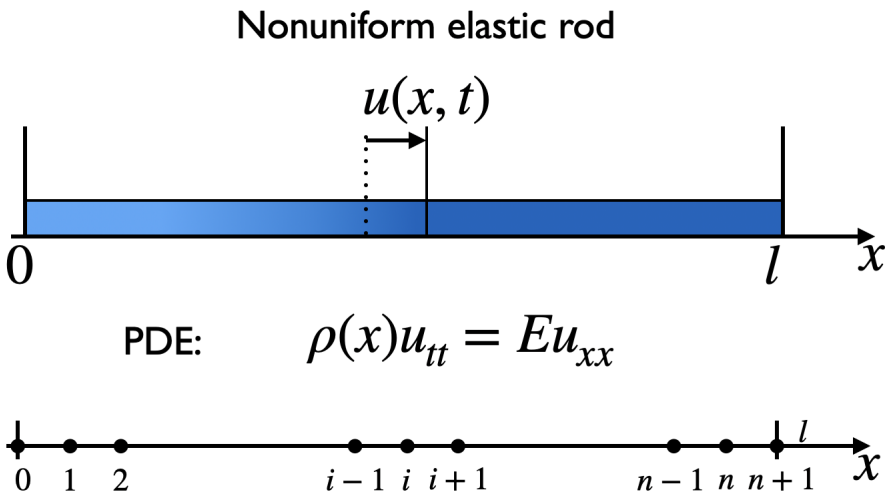

FIGURE 2.2. Longitudinal waves in an elastic rod with variable density.

2.2.4. *Boundary value problems.* We further illustrate the role of eigenvalues and eigenvectors in solving boundary value problems (BVP). More on this topic will be said in the third part of the course, and for now a simple example will suffice.

Suppose we have an elastic rod of length l, density ρ, and Young modulus E, and we consider longitudinal elastic waves in it subject to some constraints at its ends. For example, let the ends be fixed so that the displacement $u(x,t)$ of any cross section of the rod from its equilibrium position vanishes at the end points:

$$u(0,t) = u(l,t) = 0. \quad \leftarrow \text{ boundary conditions.}$$

Assuming variable density $\rho(x)$ and constant Young modulus E, the equation of motion is the wave equation:

$$u_{tt} = c^2(x)\, u_{xx}, \tag{2.12}$$

where $c^2 = E/\rho(x)$ is the square of the wave speed, which varies with x because of the variable density. The equation of motion follows from Newton's law written for an element of the rod with the forces acting on that element given by Hooke's law:

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x} = \frac{\partial}{\partial x}(E\epsilon) = \frac{\partial}{\partial x}\left(E\frac{\partial u}{\partial x}\right).$$

Equation (2.12) has separable solutions of the form $u = T(t)\,\phi(x)$ (this is the key idea behind Fourier analysis of partial differential equations). If we substitute this into the wave equation, we get

$$\ddot{T}\phi = c^2(x)\, T\phi''$$
$$\frac{\ddot{T}}{T} = \frac{c^2(x)\,\phi''}{\phi} = const = -\omega^2.$$

The time dependence here is given in terms of sines and cosines, provided ω is real and nonzero:

$$T(t) = a\cos(\omega t) + b\sin(\omega t).$$

The spatial part solves

$$c^2(x)\,\phi'' + \omega^2\phi = 0 \tag{2.13}$$

together with the homogeneous boundary conditions

$$\phi(0) = \phi(l) = 0.$$

Notice the following fact: $\phi(x) = 0$ is always a solution of the BVP. We need a nontrivial solution, and this will require some special conditions on ω. Hence this becomes an eigenvalue problem.

We can rewrite the problem so that it looks like the matrix problem we have been investigating so far. Let

$$L = -c^2(x)\,\frac{d^2}{dx^2}$$

denote the differential operator in (2.13). Then the BVP becomes

$$L\phi = \omega^2\phi$$
$$\phi(0) = \phi(l) = 0,$$

which is exactly the eigenvalue problem for L. Unlike the matrix case, however, the differential operator L comes with its boundary conditions. Different boundary conditions will lead to different answers for the same L.

Even though our interest here is the variable-speed case, let us first look at $c = const$ to get an idea of what can happen. Then the BVP

$$\phi'' + \left(\frac{\omega}{c}\right)^2\phi = 0, \quad \phi(0) = \phi(l) = 0,$$

is solved by

$$\phi = \sin(kx), \text{ where } k = \frac{\omega}{c}$$

for all k such that $\sin(kl) = 0$, i.e.

$$k = k_n = \frac{\pi n}{l},\ n = 1, 2, ...$$

Indeed, the general solution for ϕ would be $\phi = \alpha\cos(kx) + b\sin(kx)$, which at the boundaries has to vanish. Then $\phi(0) = \alpha = 0$ and $\phi(l) = b\sin(kl) = 0$. We cannot take $b = 0$ here since then the solution would be trivial, hence we must have $\sin(kl) = 0$.

And therefore, there is an infinite sequence of solutions given by

$$\phi_n(x) = \sin\left(\frac{\pi n x}{l}\right), \quad n = 1, 2, ...$$

These are eigenfunctions or the normal modes, and the corresponding time frequencies are obtained by solving the time part as

$$\omega_n = ck_n = \frac{\pi c}{l}n, \quad n = 1, 2, ...$$

The fundamental mode $n = 1$ is the half-sine $\phi_1 = \sin(\pi x/l)$ and it oscillates in time with fundamental frequency $\omega_1 = \pi c/l$. All other modes are shorter and oscillate faster. The general solution of the wave equation will be a superposition of all such normal modes just like in the case of beads on a ring. We will postpone the details of how to get that until the third part of the course.

Now, the question is: *can we find the modes for a rod that is not uniform?* The trouble is that now the differential equation $\phi'' + k^2(x)\phi = 0$ cannot be solved easily in an analytical form. So we want to solve it numerically. How do we do it? Answer: we discretize carefully and reduce the problem to a matrix form. Here are the details.

First, divide the domain $0 \le x \le l$ into $n+1$ equal parts as $x_i = ih$, $i = 0, 1, 2, ..., n+1$ and $h = l/(n+1)$. Then, $x_0 = 0$ and $x_{n+1} = l$. The goal is now to find the solution not at every point $x \in (0, l)$, but only at these discrete points x_i. And, if we have many of these points, we hope to have found the solution with good enough accuracy. This is the basic hope of any numerical method.

Since we know the solution at the boundaries $x_0 = 0$ and $x_{n+1} = l$ to be $\phi = 0$, we only need to find the solution at the n internal points $x_1, x_2, ..., x_n$. We know that at every x in the interval $(0, l)$, the solution satisfies $\phi'' + k^2(x)\phi = 0$. This equation is also satisfied at x_i, and so we evaluate the equation at $x = x_i$:

$$\begin{aligned} \phi'' + k^2(x)\phi = 0 \quad &\leftarrow \text{ at every } x \\ (\phi'')_{x_i} + k^2(x_i)\phi(x_i) = 0 \quad &\leftarrow \text{ at discrete points } x_i. \end{aligned} \tag{2.14}$$

Now, call $k(x_i) = k_i$, $\phi(x_i) = \phi_i$ and approximate the second derivative here using finite differences as

$$(\phi'')_{x_i} \approx \frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{h^2}.$$

Then (2.14) becomes

$$\phi_{i-1} - 2\phi_i + \phi_{i+1} + h^2 k_i^2 \phi_i = 0, \quad i = 1, 2, ..., n. \tag{2.15}$$

Notice that at $i = 1$ and $i = n$, we need to know ϕ_0 and ϕ_{n+1}, which are both zeros due to the boundary conditions. Therefore, at the end points the equation (2.15) gives

$$-2\phi_1 + \phi_2 + h^2 k_1^2 \phi_1 = 0, \tag{2.16}$$

$$\phi_{n-1} - 2\phi_n + h^2 k_n^2 \phi_n = 0. \tag{2.17}$$

In equations (2.15)-(2.17), we replace $k_i = \omega/c_i$, and rearrange them as

$$\begin{aligned} 2\phi_1 - \phi_2 &= \omega^2 \frac{h^2}{c_1^2}\phi_1, \quad i = 1 \\ -\phi_{i-1} + 2\phi_i - \phi_{i+1} &= \omega^2 \frac{h^2}{c_i^2}\phi_i, \quad i = 2, 3, ..., n-1 \\ -\phi_{n-1} + 2\phi_n &= \omega^2 \frac{h^2}{c_n^2}\phi_n, \quad i = n \end{aligned}$$

and then put in matrix form as

$$\underbrace{\begin{bmatrix} 2 & -1 & 0 & \cdots & \\ -1 & 2 & -1 & 0 & \\ 0 & -1 & 2 & -1 & 0 \\ \vdots & & \ddots & & -1 \\ & & & -1 & 2 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{bmatrix}}_{\phi} = \omega^2 \underbrace{\begin{bmatrix} h^2/c_1^2 & 0 & & \cdots & \\ 0 & h^2/c_2^2 & 0 & & \\ & 0 & h^2/c_3^2 & 0 & \\ \vdots & & \ddots & & 0 \\ & & & 0 & h^2/c_n^2 \end{bmatrix}}_{K} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{bmatrix}.$$

This is

$$A\phi = \omega^2 K\phi,$$

which is the generalized eigenvalue problem for eigenvalues ω^2. Since K is simple here, we can move it to the left to get the regular eigenvalue problem

$$B\phi = \omega^2 \phi,$$

where $B = K^{-1}A$, and so ω^2 are the eigenvalues of B. And so finding the oscillation frequencies of the rod reduces to finding the eigenvalues of B, which is not too much more complicated than the uniform case.

The vector ϕ is the sample of the eigenfunction $\phi(x)$ on the grid, hence it should show the shape of the eigenfunctions, like the sines $\sin(n\pi x/l)$ in the uniform case above. Except now these may be complicated looking functions depending on how the rod density varies with x.

2.3. **Singular Value Decomposition:** $A = U\Sigma V^T$ ..... SVD can be constructed for any rectangular matrix A. The idea behind the factorization can be stated as follows. Any given matrix A has r (r is the rank) independent columns which span the column space, $C(A)$, and r independent rows which span the row space, $R(A)$. In each subspace we can choose an orthonormal basis, with orthonormal basis vectors $\mathbf{u}_1$, $\mathbf{u}_2$, ..., $\mathbf{u}_r$ in $C(A)$ and $\mathbf{v}_1$, $\mathbf{v}_2$, ..., $\mathbf{v}_r$ in $R(A)$. Now we ask: Can we choose these bases so that

$$Av_1 = \sigma_1 u_1,\ Av_2 = \sigma_2 u_2, ..., Av_r = \sigma_r u_r? \tag{2.18}$$

Or

$$Av_i = \sigma_i u_i?$$

If yes, what are the constants σ_i and what are these basis vectors? Note that the question arises naturally from the desire to extend the basis properties of eigenvectors of a square matrix. If A is full rank $n \times n$ matrix, then its eigenvectors form a basis of $\mathbf{R}^n$ with nice properties. Any vector in that basis, $x = x_1 s_1 + x_2 s_2 + ...x_n s_n$ when multiplied by A gives $y = Ax = x_1\lambda_1 s_1 + x_2\lambda_2 s_2 + ...x_n\lambda_n s_n$ so that the new components are simply multiples of the old ones with the eigenvalues; A acts like a diagonal matrix in this basis.

Eq. (2.18) can be written in matrix form as

$$AV = U\Sigma$$

with v_i as columns of V, u_i as columns of U and σ_i as diagonal elements of the diagonal matrix Σ. Note that for now (see the note below) A is m by n, V is n by r, U is m by r, and Σ is r by r. We now find that

$$A = U\Sigma V^T, \tag{2.19}$$

since $VV^T = I$.

Reduced SVD:

$$A_{m\times n} = U_{m\times r}\Sigma_{r\times r}\left(V^T\right)_{r\times n} = \underbrace{\begin{bmatrix} | & | & | & | \\ u_1 & u_2 & \dots & u_r \\ | & | & | & | \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} - & v_1^T & - \\ - & v_2^T & - \\ & \vdots & \\ - & v_r^T & - \end{bmatrix}}_{V^T}$$

Here

$$u_i = \begin{bmatrix} u_{i1} \\ u_{i2} \\ \vdots \\ u_{im} \end{bmatrix} \in \mathbb{R}^m, \quad v_i = \begin{bmatrix} v_{i1} \\ v_{i2} \\ \vdots \\ v_{in} \end{bmatrix} \in \mathbb{R}^n,$$

To determine what U, Σ, and V are, we look at the symmetric matrices A^TA and AA^T:

$$A^TA = \left(U\Sigma V^T\right)^T U\Sigma V^T = V\Sigma^2 V^T,$$

$$AA^T = U\Sigma V^T\left(U\Sigma V^T\right)^T = U\Sigma^2 U^T,$$

which are just spectral factorizations of these symmetric matrices and therefore the columns of V are the eigenvectors of A^TA, columns of U are the eigenvectors of AA^T, and the "singular

values", σ_i, are the square roots of the eigenvalues of A^TA (and AA^T) which are always positive or zero.

Note: for full SVD, V is complemented with $n-r$ columns that make the null space of A, so that V becomes n by n, U is complemented with $m-r$ columns that make the left null space of A, so that U becomes m by m, and Σ is made m by n by adding zero diagonal elements below the first r non-zero σ's. Thus, SVD factorization exhibits the column space, $C(A)$, in the first r columns of U and the left null space, $N\left(A^T\right)$, in the remaining $m-r$ columns. The row space, $R(A)$, is the first r columns of V and null space, $N(A)$, the remaining $n-r$ columns of V. The rank r is equal to the number of non-zero diagonal elements of $\mathbf{\Sigma}$. The fundamental theorem of linear algebra is all in the SVD.

Full SVD:

$$A_{m\times n} = U_{m\times m}\Sigma_{m\times n}\left(V^T\right)_{n\times n} =$$

$$= \underbrace{\begin{bmatrix} | & | & | & | & & | \\ u_1 & u_2 & \dots & u_r & u_{r+1} & \dots & u_m \\ | & | & | & | & & | \end{bmatrix}}_{U_{m\times m}} \underbrace{\begin{bmatrix} \sigma_1 & & & & & \\ & \sigma_2 & & & 0 & \\ & & \ddots & & & \\ & & & \sigma_r & & \\ & & & & 0 & \\ & & & & & \ddots \\ & 0 & & & & 0 \\ & & & & & \vdots \\ & & & & & 0 \end{bmatrix}}_{\Sigma_{m\times n}} \underbrace{\begin{bmatrix} - & v_1^T & - \\ - & v_2^T & - \\ & \vdots & \\ - & v_r^T & - \\ - & v_{r+1}^T & - \\ & \vdots & \\ - & v_n^T & - \end{bmatrix}}_{V^T_{n\times n}}$$

So, the blue columns of U span the $m-r$ dimensional nullspace of A^T, and the blue rows of V^T span the $n-r$ dimensional nullspace of A.

This follows from looking at $Av_0 = U\Sigma V^Tv_0 = 0$ for the nullspace of A. Since $U\Sigma V^T$ is a matrix with rows which are combinations of rows of V^T, then $U\Sigma V^Tv_0 = 0$ implies that v_0 is orthogonal to all the rows of this matrix, and hence to all the rows of V^T. So the nullspace of A is orthogonal to the rows of V^T or to the columns of V.

Similar reasoning holds for the left nullspace.

We can write Eq. (2.19) as a sum of outer products of the basis vectors (a sum of rank one matrices):

$$A = \sigma_1u_1v_1^T + \sigma_2u_2v_2^T + ... + \sigma_ru_rv_r^T$$

If the singular values are arranged in decreasing order, $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_r$, then one can use the above decomposition in order to approximate large matrices by simply discarding terms with σ_i smaller than a given value, in hope that the larger singular values and corresponding basis vectors sufficiently accurately represent the essential nature of A. Then this is a low-rank approximation of A.

Example: Compute SVD of

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 0 \end{bmatrix}.$$

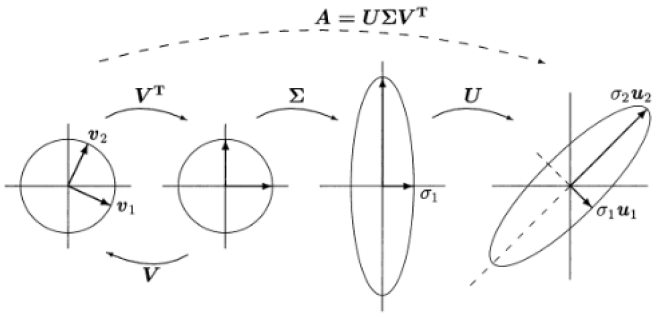

FIGURE 2.3. Geometry of SVD.

Note that A is a rank one matrix. We need the eigenvalues and eigenvectors of A^TA and AA^T to construct U, V, and $\mathbf{\Sigma}$:

$$A^TA = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}, \quad AA^T = \begin{bmatrix} 5 & 0 \\ 0 & 0 \end{bmatrix}.$$

Therefore, $\sigma_1 = \sqrt{5}$ is the only singular value and hence

$$\Sigma = \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 0 \end{bmatrix}.$$

The eigenvalues and normalized eigenvectors of A^TA are

$$\lambda_1 = 5: \quad v_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad \lambda_2 = 0: \quad v_2 = \frac{1}{\sqrt{5}} \begin{bmatrix} -2 \\ 1 \end{bmatrix},$$

and those of AA^T are

$$\lambda_1 = 5: \quad u_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \lambda_2 = 0: \quad u_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

so that

$$U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad V = \begin{bmatrix} \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}$$

and the final result is

$$A = U\Sigma V^T = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix},$$

which can also be written as the outer product $\sigma_1 u_1 v_1^T$:

$$A = \sqrt{5} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \end{bmatrix}.$$

Note that the first column of U spans the column space of A, the second column spans the left null space, while the first column of V spans the row space of A and the second column of V spans the null space of A. One can check the orthogonality of these subspaces as stated in the fundamental theorem: $C(A) \perp N\left(A^T\right)$, $R(A) \perp N(A)$.