18.085/18.0851 Computational Science and Engineering I **Summer 2020**

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3.1 Positive Definite, Negative Definite, Semi-definite, and Indefinite Matrices

While numbers are easier to assign a positive or negative sign, matrices are not. What exactly do we mean by a positive or negative matrix? More fundamentally, why do we even care to define such notions for matrices? In this section, we shall present the definiteness of matrices. First we define what it is

Definition 3.1 *$A \in \mathbb{R}^{n\times n}$ is a positive definite matrix if the quadratic form, $u^TAu > 0$, for every vector $u \in \mathbb{R}^n$.*

Equivalently, we can also introduce negative definite, semidefinite, indefinite matrices

Definition 3.2 *$A \in \mathbb{R}^{n\times n}$ is a positive or negative semi-definite matrix if the quadratic form, $u^TAu \geq 0$ or $u^TAu \leq 0$, respectively, for every vector $u \in \mathbb{R}^n$.*

Definition 3.3 *$A \in \mathbb{R}^{n\times n}$ is a indefinite matrix if the quadratic form, u^TAu, can have any sign, where $u \in \mathbb{R}^n$.*

Let's get a feeling of what each of each type of matrices really entails

3.1.1 Positive/Negative Definite

Here is a useful fact that you might already have discovered from the previous homework

Theorem 3.4 *If a matrix is positive/negative definite, then all of their eigenvalues are positive/negative.*

A classic example of a positive definite matrix is the second derivative finite difference matrix, K. Let's multiply out the matrix by an arbitrary vector $u = [u_1, u_2]^T$.

$$\begin{bmatrix} u_1 & u_2 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = 2u_1^2 + 2(u_1 - u_2)^2 + 2u_2^2 \tag{3.1}$$

The quadratic form is never nonpositive.

3.1.2 Semidefinite Matrix

Theorem 3.5 *If a matrix is positive/negative semidefinite, then all of their eigenvalues are non-negative/non-positive.*

Let's take B, defined as.

$$B = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{3.2}$$

Let's multiply out the matrix by an arbitrary vector $u = [u_1, u_2]^T$.

$$\begin{bmatrix} u_1 & u_2 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = (u_1 - u_2)^2 \tag{3.3}$$

Notice that the quadratic can be either zero or positive.

3.1.3 Indefinite matrix

Theorem 3.6 *The eigenvalues of an indefinite matrix can have any signs.*

Let's take M,

$$M = \begin{bmatrix} 1 & -3 \\ -3 & 1 \end{bmatrix} \tag{3.4}$$

Multiplying out the quadratic form, we have

$$\begin{bmatrix} u_1 & u_2 \end{bmatrix} \begin{bmatrix} 1 & -3 \\ -3 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = (u_1 - 3u_2)^2 - 8u_2^2 \tag{3.5}$$

Notice that the quadratic form can take any signs, depending on the vector u.

Here is another nice fact about positive, definite, symmetric matrices

Theorem 3.7 *Let $A \in \mathbb{R}^{n \times n}$ be a positive, definite symmetric matrix. Then all eigenvalues of A are positive and real. All eigenvectors are orthogonal.*

3.1.4 A Quick Note about Positive, Definite, Symmetric (PSD) Matrices

Positive, definite, symmetric matrices enjoy the nice property that all of their eigenvalues are positive and real and all of their eigenvectors are orthogonal to each other. If all eigenvectors are orthogonal, we can normalize them to make them orthonormal. Then when we formulate the diagonalized matrix, V, V becomes an orthogonal matrix (with orthonormal columns). Here is a nice property of orthogonal matrices

Theorem 3.8 *Let $A \in \mathbb{R}^{n \times n}$ be an orthogonal matrix. Then $A^{-1} = A^T$*

3.1.5 Second Derivative Test for Higher Dimension

Here is an application of positive definite matrices. Let $f(x_1, ..., x_n) : \mathbb{R}^n \to \mathbb{R}$ be a smooth function. Then we can introduce the Hessian matrix, $H \in \mathbb{R}^{n \times n}$, as

$$H_{ij} = H_{ij} = \frac{\partial f^2}{\partial x_i \partial x_j} \tag{3.6}$$

Theorem 3.9 *Let $f(x_1, ..., x_n) : \mathbb{R}^n \to \mathbb{R}$ be a smooth function and let H be the Hessian matrix defined at a critical point, x, ie. $\nabla f(x) = 0$. Then*

- *If $H(x)$ is positive definite, then x is a local minimum*
- *If $H(x)$ is negative definite, then x is a local maximum*
- *If $H(x)$ is indefinite, then x is a saddle point*
- *If $H(x)$ is semidefinite, then the test is inconclusive.*

3.2 Matrix Decomposition: SVD, QR, and LU

Matrix decomposition refers to ways to rewrite a matrix as the product of several matrices. The diagonalization of A, $A = V\Lambda V^{-1}$ is a form of matrix decomposition. However, the ability to diagonalize a matrix completely depends on whether all of A's eigenvectors are linearly independent or not. Plus, the concept ceases to make sense for non-square matrices. Hence, we need additional methods to decompose a matrix. The most popular three include

- QR factorization: $A = QR =$ orthogonal times upper triangular
- LU decomposition: $A = LU =$ lower triangular times upper triangular
- Singular Value Decomposition (SVD): $A = U\Sigma V^T =$ orthogonal matrix * singular values * orthogonal matrix

For this lecture, we will only talk about SVD. You can find information about the other decompositions in the textbook.

3.2.1 The Mechanics of SVD

For $A \in \mathbb{R}^{m\times n}$, $A = U\Sigma V^T$ has the following properties

- $U \in \mathbb{R}^{m\times m}$ the eigenvector matrix of AA^T
- $V \in \mathbb{R}^{n\times n}$ the eigenvector matrix of A^TA
- $\Sigma \in \mathbb{R}^{m\times n}$ the diagonal matrix whose values on the diagonal equal the square roots of the eigenvalues of A^TA

Let's do SVD on A defined as below

$$A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix} \tag{3.7}$$

3.2.1.1 Step 1: Compute A^TA and AA^T

We compute

$$A^TA = \begin{bmatrix} 13 & 12 & 2 \\ 12 & 13 & -2 \\ 2 & -2 & 8 \end{bmatrix} \tag{3.8}$$

$$AA^T = \begin{bmatrix} 17 & 8 \\ 8 & 17 \end{bmatrix} \tag{3.9}$$

3.2.1.2 Step 2: Compute the eigenvalues of A^TA or AA^T

Since the eigenvalues of A^TA are much easier to compute than those of AA^T, we compute the eigenvalues of A^A and obtain that $\lambda_1 = 25$, $\lambda_2 = 9$.
The eigenvalues of AA^T should then be $25, 9$ and 0.

3.2.1.3 Step 3: Compute the eigenvectors of A^TA or AA^T and stack them up into U and V matrices

We compute the eigenvectors of A^TA and AA^T before stacking them up side by side into U and V. Note that they must be normalized. As such,

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}, V = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{18}} & -\frac{1}{\sqrt{18}} & \frac{4}{\sqrt{18}} \\ \frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} \end{bmatrix} \tag{3.10}$$

3.2.1.4 Step 4: Write everything down

We then conclude that $A = U\Sigma V^T$, where

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}, \Sigma = \begin{bmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix}, V^T = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{18}} & -\frac{1}{\sqrt{18}} & \frac{4}{\sqrt{18}} \\ \frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} \end{bmatrix} \tag{3.11}$$

3.2.1.5 Application of SVD: Image Process

All images are made of pixels, which we can convert to matrices. The singular values of the matrix captures the key information about an image. "Killing" some of the singular values would effectively reduce some of the information, making the image "blurry". See the code demonstration for more details.

3.3 Numerical Linear Algebra

This section is a short introduction to numerical linear algebra. As there is a whole separate course on it, we cannot get into the details of many topics. The purpose is to give you a flavor of the subject and get familiar with some of the terminology and algorithm used in the various scientific and engineering subjects.

A large-if not entire-chunk of numerical linear algebra-is concerned with solving linear systems of $Ax = b$. However, often time, A is not a square matrix. This begs the question of what it means to solve $Ax = b$, for which we introduce the concept least square

3.3.1 Least Square Problem

Definition 3.10 *For any matrix $A \in \mathbb{R}^{m\times n}$ and $b \in \mathbb{R}^m$, x is the solution to the least square problem $Ax = b$ if $u = x$ minimizes $||b - Au||^2$, for all $u \in \mathbb{R}^n$ Analytically, we can derivative that the least-square estimate is the solution to the normal equation*

$$A^T Au = A^T b \tag{3.12}$$

where $A^T A$ is a square symmetric matrix and therefore is invertible.

Here is an example: suppose that we have measurements $b = 1, 9, 9, 21$ at four positions $x = 0, 1, 3, 4$. We believe that the relation between the position and measurements are linearly related, and therefore proposes the linear relation $y = C + Dx$. Then we can formulate the equation

$$\begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 1 \\ 9 \\ 9 \\ 21 \end{bmatrix} \tag{3.13}$$

Solving the normal equation, we obtain that $C = 2$ and $D = 4$.

3.3.2 QR Factorization

Described as one of the most important algorithms in numerical linear algebra, the QR factorization factors a square matrix A into an orthogonal matrix Q and an upper triangular matrix R. Once QR is complete, we can then solve the original linear problem via

$$Ax = b \tag{3.14}$$
$$QRx = b \tag{3.15}$$
$$Rx = Q^T b \tag{3.16}$$

the last line of which can be solved using backward substitution. Additionally, it can also solve the least square problem by solving the normal equation $A^T Au = A^T b$ via

$$(QR)^T QRu = (QR)^T b \tag{3.17}$$
$$R^T Ru = R^T Q6Tb \tag{3.18}$$
$$Ru = Q^T b \tag{3.19}$$

Since R is upper triangular, we can solve the linear system in the last line using backward substitution. The key is how to generate the matrices Q and R. To that end, we would like to present the Gram-Schmidt algorithm

3.3.2.1 Gram-Schmidt Algorithm

The Gram-Schmidt algorithm gives a simple construction of the columns of Q (denoted as q_i for the i^{th} column) from the columns of A (denoted as a_i for the i^{th} column). To obtain Q, we perform

$$u_1 = a_1, q_1 = \frac{u_1}{||u_1||} \tag{3.20}$$

$$u_2 = a_2 - \frac{u_1 \cdot a_2}{u_1 \cdot u_1} q_1, q_2 = \frac{u_2}{||u_2||} \tag{3.21}$$

$$u_3 = a_3 - \frac{u_1 \cdot a_3}{u_1 \cdot u_1} q_1 - \frac{u_2 \cdot a_3}{u_2 \cdot u_2} q_2, q_3 = \frac{u_3}{||u_3||} \tag{3.22}$$

$$\dots \tag{3.23}$$

$$u_k = a_k - \sum_{j=1}^{k-1} \frac{a_k \cdot u_j}{u_j \cdot u_j} q_j, q_k = \frac{u_k}{||u_k||} \tag{3.24}$$

Once the columns of Q are obtained, we can proceed with calculating $R = Q^T A$.

This numerical scheme turns out to be unstable due to round-off errors. To make them stable, we will need a slightly *modified* Gram-Schmidt algorithm. We will not cover it in this class.

3.3.3 Condition Number

The condition number of a matrix A characterizes the sensitivity of the linear system $Ax = b$. In other words, if I change b by a small amount, eg. Δb, how much do I change x, ie. how big is Δx. The condition tries to capture the multiplier on Δx as a result of Δb. By definition,

Definition 3.11 *The condition number of a matrix A, denoted as $\kappa(A)$ or $c(A)$, is defined as:* $\kappa(A) = ||A||||A^{-1}||$

where $||A||| = \max_{||x||=1} ||Ax||$ is also known as the norm of the matrix. This definition, however, is often not very convenient in computing the actual condition number of the matrix. It is more common to use the derived notion of condition number as

$$\kappa(A) = \frac{\text{Largest Singular Value}}{\text{Smallest Singular Value}} \tag{3.25}$$

As an example, suppose we have the following matrix

$$A = \begin{bmatrix} 1 & 7 \\ 0 & 1 \end{bmatrix} \tag{3.26}$$

and the vector

$$b = \begin{bmatrix} 7 & 1 \end{bmatrix} \tag{3.27}$$

Solving $Ax = b$, we obtain that $x = [0, 1]^T$. Now we shift b by $[0, 0.1]^T$ and let $b_2 = [7, 0.9]^T$. Then we obtain that $x_2 = [-6.3, 0.9]^T$. We compute

$$\frac{||\Delta x||}{||x||} = 0.1\sqrt{50} \tag{3.28}$$

$$\frac{||\Delta b||}{||b||} = \frac{0.1}{\sqrt{50}} \tag{3.29}$$

So a little change in b triggers the solution to change by a factor of 50.

Roughly speaking, in solving $Ax = b$, the computer loses $log(\kappa(A))$ number of digits. It is common for the condition number of a second difference matrix to be on the scale of $O(1/\Delta x^2)$. This is why a finer mesh does not always lead to a more accurate answer. Once the condition number gets too large, various sources of errors start amplifying their effects, rendering the entire solution garbage.

3.4 A Quick Note about Errors

There are two types of errors in numerical methods:

- Round-off error: errors that occur due to finite representation of series.

- Floating point error: errors that occur due to finite representations of numbers

Both contribute to the errors of our numerical methods. It is therefore crucial that our methods remain stable. We will talk further about what they mean in the future. For now, here are a few tips when implementing numerical algorithms

- Avoid subtracting two very small numbers
- Avoid adding or multiplying very large numbers

3.5 Equilibrium and the Stiffness Matrix

We are moving into a new chapter on a general framework for applied mathematics. There are a wide range of applications. For this lecture, we are focusing on the spring-mass system, one of the simplest models in mathematics and physics that nonetheless finds itself everywhere in natural and engineering problems, from fluid mechanics to quantum mechanics.

3.5.1 A Line of Spring

Imagine three masses hung vertically from the ceiling and connected by springs. While the top mass m_1 is fixed from the ceiling, the bottom mass m_2 may be fixed to the ground or hung freely (in which case there is no spring). The former is known as the fixed-fixed end, while the latter is called the fixed-free end. You will explore the latter in the homework.

Our goal is to related the displacement of each mass, $u = (u_1, u_2, u_3)^T$ with the external force on each mass, $f = (f_1, f_2, f_3)^T$. To go from displacement of masses to their external forces, we must jump through elongations of springs and the internal forces in the springs. In summary, we have

- $u =$ displacement of n masses
- $e =$ elongations of m springs

- w = Internal forces in m springs
- f = External forces on n masses

Here are the steps

3.5.1.1 Step 1: Displacement → Elongations

The elongation e refers to how far the springs are extended. Once the springs are hung vertically, gravity starts pulling down and the masses fall by u_1, u_2, and u_3. If mass 2 drops by u_2 and mass 1 drops by u_1, the spring stretches by $u_2 - u_1$, whence

$$e_1 = u_1 \tag{3.30}$$
$$e_2 = u_2 - u_1 \tag{3.31}$$
$$e_3 = u_3 - u_2 \tag{3.32}$$
$$e_4 = -u_3 \tag{3.33}$$

We can then write down the matrix equation

$$\begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \tag{3.34}$$

Let's call this matrix A.

3.5.1.2 Step 2: Elongations → Internal Forces

The equation that connects the forces in the springs with elongations is empirical, known as the Hooke's law. It says that the force of a spring is proportional to its elongation, and the proportionality constant is known as the spring constant. Let c_i be the spring constant of the i^{th} spring. We then know that $w_i = c_i e_i$, whence

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} c_1 & 0 & 0 & 0 \\ 0 & c_2 & 0 & 0 \\ 0 & 0 & c_3 & 0 \\ 0 & 0 & 0 & c_4 \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix} \tag{3.35}$$

Let's call this matrix C.

3.5.1.3 Step 3: Internal Forces → External Forces

Finally, we know that the forces need to balance, ie. the internal and external forces have to balance. Since each mass is in equilibrium, pulled up by a spring of force w_j and down by w_{j+1}, the external force on mass j, f_j, must be $f_j = w_j - w_{j+1}$, whence

$$f_1 = w_1 - w_2 \tag{3.36}$$
$$f_2 = w_2 - w_3 \tag{3.37}$$
$$f_3 = w_3 - w_4 \tag{3.38}$$
$$\tag{3.39}$$

We can then write down the matrix equation

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} u_1 - 0 \\ u_2 - u_1 \\ u_3 - u_2 \\ 0 - u_3 \end{bmatrix} \tag{3.40}$$

This matrix is exactly A^T.

3.5.1.4 Step 4: Putting everything together

To relate f with u, we multiply everything above together and obtain that

$$f = A^T C A u \tag{3.41}$$

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} c_1 & 0 & 0 & 0 \\ 0 & c_2 & 0 & 0 \\ 0 & 0 & c_3 & 0 \\ 0 & 0 & 0 & c_4 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \tag{3.42}$$

We call the matrix $K = A^T C A$ the stiffness matrix of the system. When $C = I_3$, K becomes exactly the second difference matrix of dimension 3. Therefore, we can conclude that

$$u = K^{-1} f \tag{3.43}$$

Here are some nice properties of K

- K is tridiagonal, because mass 3 is not connected with mass 1
- K is symmetric, because C is symmetric
- K is positive definite, because A has independent columns
- K^{-1} is a full matrix with all positive entries

For our example above, assume that $c_i = c$ and $m_i = m$ (ie. all springs and masses are identical). Since gravity is the only external force, we let $f = (mg, mg, mg)$, whence,

$$u = K^{-1} f \tag{3.44}$$

$$= \frac{1}{4c} \begin{bmatrix} 3 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} mg \\ mg \\ mg \end{bmatrix} \tag{3.45}$$

$$= \frac{mg}{c} \begin{bmatrix} 1.5 \\ 2.0 \\ 1.5 \end{bmatrix} \tag{3.46}$$

We can also compute the elongation vector using $e = Au$

$$\begin{aligned} e &= Au \qquad (3.47) \\ &= \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{bmatrix} \frac{mg}{c} \begin{bmatrix} 1.5 \\ 2.0 \\ 1.5 \end{bmatrix} \qquad (3.48) \\ &= \frac{mg}{c} \begin{bmatrix} 1.5 \\ 0.5 \\ -0.5 \\ -1.5 \end{bmatrix} \qquad (3.49) \end{aligned}$$

Note that all elongations add up to 0, which makes sense since both ends are fixed.

3.6 Inverted Pendulum

Let's examine the problem of an inverted pendulum with a spring attached to the connecting rod. We can write down the total energy as

$$P(u) = \frac{1}{2}c\theta^2 + mgL\cos(\theta) \qquad (3.50)$$

Hence, equilibrium is achieved when $\frac{dP}{d\theta} = c\theta - mgL\sin(\theta) = 0$.

Note that $\theta = 0$ is always a solution. The questions are

- Is the solution stable?
- Are there other solutions?
- If so, are they stable?

To answer the first question, we run the second derivative test by computing

$$\frac{d^2P}{d\theta^2}c - mgL\cos(\theta) \qquad (3.51)$$

This value is positive when $c > mgL$ and negative when $c < mgL$. Since positive second derivatives indicate local minimum, $\theta = 0$ is stable for $c > mgL$. When the pendulum is too light and/or the spring is too strong, the ball just sits on top nicely.

The second question can be answered by realizing that $dP/d\theta$ can also achieve zero away from $\theta = 0$ when $c/mgL < 1$. In which case, $\theta = 0$ becomes unstable along with the rise of two new critical points θ^* such that $mgL\sin(\theta^*) = c\theta^*$. The two θ^* can be calculated numerically to render positive second derivatives, which suggests that the new critical points are local minima.

The transition from one stable minimum at the origin to a unstable solution with two new stable solutions is called "pitchfork bifurcations", or second-order phase transitions by physicists. It is a ubiquitous process found everywhere in nature, from classical mechanics to quantum mechanics.