Chapter 6

Matrix Analysis

Coupled linear equations of N variables

$$\mathsf{A}\mathsf{x} = \mathsf{b} \tag{6.1}$$

with an $N \times N$ matrix for coefficients A_{ij}

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2N} \\ \vdots & \vdots & \vdots & \ddots & \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN} \end{pmatrix}, \tag{6.2}$$

and $N \times 1$ column vectors for variables x_i and constants b_i

$$\mathsf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_N \end{pmatrix}, \qquad \mathsf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_N \end{pmatrix}. \tag{6.3}$$

Second order differential equation

$$\frac{d^2 y(x)}{dx^2} + k^2(x) y(x) = S(x) \tag{6.4}$$

in a discretized grid space $x_1, x_2, \cdots, x_N$ with a grid spacing of h can be expressed by a matrix equation with

$$
\mathsf{A} = \begin{pmatrix}
-\frac{2}{h^2}+k_1^2 & \frac{1}{h^2} & 0 & 0 & \cdots & & & \\
\frac{1}{h^2} & -\frac{2}{h^2}+k_2^2 & \frac{1}{h^2} & 0 & \cdots & & & \\
0 & \frac{1}{h^2} & -\frac{2}{h^2}+k_3^2 & \frac{1}{h^2} & \cdots & & & \\
\vdots & \ddots & \ddots & \ddots & \ddots & & & \\
 & & & \cdots & 0 & \frac{1}{h^2} & -\frac{2}{h^2}+k_{N-1}^2 & \frac{1}{h^2} \\
 & & & \cdots & 0 & 0 & \frac{1}{h^2} & -\frac{2}{h^2}+k_N^2
\end{pmatrix},
$$

$$
\mathsf{x} = \begin{pmatrix} y(x_1) \\ y(x_2) \\ y(x_3) \\ \vdots \\ y(x_{N-1}) \\ y(x_N) \end{pmatrix}, \qquad
\mathsf{b} = \begin{pmatrix} S(x_1) \\ S(x_2) \\ S(x_3) \\ \vdots \\ S(x_{N-1}) \\ S(x_N) \end{pmatrix}, \tag{6.5}
$$

and $k_n = k(x_n)$. Here the $N \times N$ matrix A is a tri-diagonal matrix.

6.1 Matrix Inversion

The solution of Eq.(6.1) is

$$
\mathsf{x} = \mathsf{A}^{-1}\mathsf{b} \tag{6.6}
$$

with the inverse matrix A^{-1}. The determinant of the matrix A should be non-zero for the inverse matrix A^{-1} to exist. Inverse matrix can be found using Gauss-Jordan method: Change matrix A and unit matrix I ($I_{ij} = \delta_{ij}$) in the same way until matrix A changed to unit matrix I, i.e.,

$$
\mathsf{T_i} \cdots \mathsf{T_j T_k A} = \mathsf{I} \quad : \quad \mathsf{T_i} \cdots \mathsf{T_j T_k I} = \mathsf{A}^{-1}. \tag{6.7}
$$

The matrices $\mathsf{T_i}$ are, for 5×5 matrix as an example,

$$
\mathsf{T_1} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & a & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix},
$$

$$\mathsf{T_2} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{6.8}$$

$$\mathsf{T_3} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & b & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{pmatrix}.$$

Multiplying $\mathsf{T_i}$ to A from left

$$\mathsf{T_1A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ aA_{31} & aA_{32} & aA_{33} & aA_{34} & aA_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{pmatrix},$$

$$\mathsf{T_2A} = \begin{pmatrix} A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{pmatrix}, \tag{6.9}$$

$$\mathsf{T_3A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41}+bA_{21} & A_{42}+bA_{22} & A_{43}+bA_{23} & A_{44}+bA_{24} & A_{45}+bA_{25} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{pmatrix}.$$

Multiplying $\mathsf{T_i}$ to A from right

$$\mathsf{AT_1} = \begin{pmatrix} A_{11} & A_{12} & aA_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & aA_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & aA_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & aA_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & aA_{53} & A_{54} & A_{55} \end{pmatrix},$$

$$\mathsf{AT}_2 = \begin{pmatrix} A_{14} & A_{12} & A_{13} & A_{11} & A_{15} \\ A_{24} & A_{22} & A_{23} & A_{21} & A_{25} \\ A_{34} & A_{32} & A_{33} & A_{31} & A_{35} \\ A_{44} & A_{42} & A_{43} & A_{41} & A_{45} \\ A_{54} & A_{52} & A_{53} & A_{51} & A_{55} \end{pmatrix}, \tag{6.10}$$

$$\mathsf{AT}_3 = \begin{pmatrix} A_{11} & A_{12}+bA_{14} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22}+bA_{24} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32}+bA_{34} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42}+bA_{44} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52}+bA_{54} & A_{53} & A_{54} & A_{55} \end{pmatrix}.$$

To find the inverse matrix of A, change A and I in the same way by exchanging two rows, multiplying a constant to one row, or multiplying a constant to one row and add the result to some other row until A changed to a unit matrix I. During this process, keep diagonal element (called pivot element) non-zero by exchanging two rows or columns if necessary.

6.2 Eigenvalue Problem

For some special vector $\mathsf{x} = \phi_n$ in Eq.(6.1), the vector $\mathsf{b} = \mathsf{A}\phi_n$ becomes the vector ϕ_n times a constant λ_n. Thus, the eigenvalue equation for $N \times N$ matrix A is

$$\mathsf{A}\phi_n = \lambda_n \phi_n \tag{6.11}$$

with eigenvalue λ_n and eigenvector ϕ_n. Eigenvector ϕ_n can have an arbitrary norm and we usually normalize the norm to be 1. The determinant of $(\mathsf{A}-\lambda\mathsf{I})$ should be zero at $\lambda = \lambda_n$, i.e.,

$$P_A(\lambda) = |\mathsf{A} - \lambda \mathsf{I}| = \prod_{n=1}^{N} (\lambda_n - \lambda) = 0. \tag{6.12}$$

For a tri-diagonal matrix A,

$$P_A(\lambda) = \begin{vmatrix} A_{11}-\lambda & A_{12} & 0 & 0 & 0 & \cdots & & \\ A_{21} & A_{22}-\lambda & A_{23} & 0 & 0 & \cdots & & \\ 0 & A_{32} & A_{33}-\lambda & A_{34} & 0 & \cdots & & \\ & & \cdots & & & & & \\ & & & & \cdots & 0 & A_{NN-1} & A_{NN}-\lambda \end{vmatrix}$$

This determinant can be found recursively as

$$
\begin{aligned}
P_1(\lambda) &= A_{11} - \lambda, \\
P_2(\lambda) &= (A_{22} - \lambda)P_1(\lambda) - A_{12}A_{21}, \\
P_3(\lambda) &= (A_{33} - \lambda)P_2(\lambda) - A_{23}A_{32}P_1(\lambda), \\
\cdots \\
P_n(\lambda) &= (A_{nn} - \lambda)P_{n-1}(\lambda) - A_{nn-1}A_{n-1n}P_{n-2}(\lambda).
\end{aligned} \tag{6.13}
$$

We may need only few eigenvalues for a large N. Then use $P_n(\lambda) = 0$ with n large enough but much smaller than N.

For a symmetric or Hermitian matrix, eigenvalues are real and eigenvectors are orthogonal.

6.3 Inverse Vector Iteration

Inverse vector iteration is one of simple methods of finding eigenvector ϕ_n of a matrix A for a given eigenvalue λ_n. For the eigenvector ϕ_n of a matrix A,

$$[\mathsf{A} - (\lambda_n + \epsilon)\mathsf{I}]\,\phi_n = -\epsilon\phi_n$$

with an arbitrary constant ϵ. However if ϕ is not the eigenvector ϕ_n then

$$[\mathsf{A} - (\lambda_n + \epsilon)\mathsf{I}]\,\phi = c\phi' \neq -\epsilon\phi$$

in general. Using these facts, the eigenvector ϕ_n for a given eigenvalue λ_n of matrix A can be found iteratively as

$$\phi_n^{(2)} = C\,[\mathsf{A} - (\lambda_n + \epsilon)\mathsf{I}]^{-1}\,\phi_n^{(1)} \tag{6.14}$$

together with normalization condition. Without the relaxation parameter ϵ, inverse of $[\mathsf{A} - \lambda_n\mathsf{I}]$ does not exists for eigenvector ϕ_n.

6.4 Damped Gradient Iteration

For a matrix $\mathsf{H} = \mathsf{T} + \mathsf{V}$ with eigenvalue ω,

$$
\begin{aligned}
\psi' &= \psi - d[K_0\mathsf{I} + \mathsf{T}]^{-1}(\mathsf{H} - \omega)\psi \\
&= \psi - \epsilon[\mathsf{I} + \mathsf{T}/K_0]^{-1}(\mathsf{H} - \omega)\psi.
\end{aligned} \tag{6.15}
$$

If ψ is the eigenvector of H with eigenvalue ω, then $\psi' = \psi$. The damping constant K_0 is used to stabilize the components with small kinetic energy $\mathsf{T} = C\nabla^2$ and ϵ is a relaxation parameter. The value of K_0 must be roughly the depth of the potential V.

6.5 Lanczos Algorithm

For an arbitrary vector x, $\mathsf{x}_n = \mathsf{A}^n\mathsf{x}$ becomes eigenvector of A with largest eigenvalue for a large n. With a proper unitary matrix U, $\mathsf{A} = \mathsf{U}\mathsf{diag}(\lambda_\mathsf{i})\mathsf{U}^\dagger$ and $\mathsf{A}^n = \mathsf{U}\mathsf{diag}(\lambda_\mathsf{i}^\mathsf{n})\mathsf{U}^\dagger$.

To find some lowest eigenvalues for a large symmetric matrix, approximate a large matrix A by a tridiagonal matrix in a smaller basis space. Choose basis vectors as,

$$\begin{aligned}
&\psi_1, \\
\psi_2 &= C_2(\mathsf{A}\psi_1 - A_{11}\psi_1), \\
\psi_3 &= C_3(\mathsf{A}\psi_2 - A_{22}\psi_2 - A_{21}\psi_1), \qquad (6.16)\\
&\cdots \\
\psi_{n+1} &= C_{n+1}(\mathsf{A}\psi_n - A_{nn}\psi_n - A_{nn-1}\psi_{n-1})
\end{aligned}$$

with normalization constants of

$$\begin{aligned}
C_2 &= [(\mathsf{A}\psi_1)^t(\mathsf{A}\psi_1) - (A_{11})^2]^{-1/2}, \\
C_3 &= [(\mathsf{A}\psi_2)^t(\mathsf{A}\psi_2) - (A_{22})^2 - (A_{21})^2]^{-1/2}, \qquad (6.17)\\
&\cdots \\
C_{n+1} &= [(\mathsf{A}\psi_n)^t(\mathsf{A}\psi_n) - (A_{nn})^2 - (A_{nn-1})^2]^{-1/2}
\end{aligned}$$

where $A_{nm} = \psi_n^t\mathsf{A}\psi_m$ and ψ_{i-1}, ψ_i, and ψ_{i+1} are orthogonal. The first vector ψ_1 should not be an eigenvector of the matrix A. Then approximate the large matrix A with smaller tridiagonal matrix with elements $A_{nm} = \psi_n^t\mathsf{A}\psi_\mathsf{m}$. Using this small tridiagonal matrix, find even smaller number of eigenvectors and eigenvalues for lowest eigenvalues.

Gram-Schmidt orthogonalization of vectors. For vectors $\phi_1, \phi_2, \cdots, \phi_N$,

$$\begin{aligned}
\psi_1 &= C_1\phi_1, \\
\psi_2 &= C_2(\phi_2 - \psi_1\psi_1^t\phi_2), \\
\psi_3 &= C_3(\phi_3 - \psi_2\psi_2^t\phi_3 - \psi_1\psi_1^t\phi_3), \qquad (6.18)
\end{aligned}$$

$$
\begin{aligned}
&\dots \\
\psi_n &= C_n \left(\phi_n - \sum_{i=1}^{n-1} \psi_i \psi_i^t \phi_n \right), \\
&\dots \\
\psi_N &= C_N \left(\phi_N - \sum_{i=1}^{N-1} \psi_i \psi_i^t \phi_N \right).
\end{aligned}
$$

The new vectors ψ_n are orthonormal with proper normalization constant C_n.