Application of solving a linear system: 1-D Poisson Equation

$$\frac{d^2 V}{dx^2} = f(x)$$

V is electrostatic potential associated with a charge distribution $\rho(x)$ $\quad \left[f(x) = -\frac{\rho(x)}{\epsilon_0} \right]$

or gravitational potential with $f(x) = -4\pi G \rho(x)$, where $\rho(x)$ is mass distribution

Discretize second derivative and get

$$V_{n-1} - 2V_n + V_{n+1} = h^2 f_n$$

$$h = \Delta x \quad , \quad f_n = f(x_n) \quad , \quad n = 1, 2, \ldots N$$

$$x_0 < x_n < x_{N+1}$$

and we assume that we know

$$V_0 = V(x_0)$$
$$V_{N+1} = V(x_{N+1})$$

from boundary conditions

We get

$$\begin{array}{llllll}
n=1 & & -2V_1 & +V_2 & = & h^2 f_1 - V_0 \\
n=2 & V_1 & -2V_2 & +V_3 & = & h^2 f_2 \\
n=3 & V_2 & -2V_3 & +V_4 & = & h^2 f_3 \\
\vdots & & & & & \\
n=N & V_{N-1} & -2V_N & & = & h^2 f_N - V_{N+1}
\end{array}$$

which is a matrix equation

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 & & & & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & \cdots & & & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & & & & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & & & & 0 \\ \vdots & & & & & & & & & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & & & & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \\ \vdots \\ V_{N-1} \\ V_N \end{pmatrix} = \begin{pmatrix} h^2 f_1 - V_0 \\ h^2 f_2 \\ h^2 f_3 \\ h^2 f_4 \\ \vdots \\ h^2 f_{N-1} \\ h^2 f_N - V_{N+1} \end{pmatrix}$$

or $$A\vec{x} = \vec{b}$$

with A a tridiagonal matrix

Best to find routine specialized for tridiagonal matrices

→ avoid storing all the zeros

→ faster

show A4, Q1

show code for Poisson problem

Note: In 2D we have $V_{m,n-1} + V_{m,n+1} + V_{m-1,n} + V_{m+1,n} - 4V_{m,n} = h^2 f_{m,n}$

Can map matrix of unknowns ($V_{m,n}$'s) to a vector $\hat{V}_i$ via "dictionary orders"

$(m,n) =$	$(1,1)$	$(1,2)$	$\ldots (1,N)$	$(2,1)$	$(2,2)$	$\ldots (2,N)$	$\ldots (N,1)$	$\ldots$	(N,N)
$i =$	1	2	N	$N+1$	$N+2$	$2N$	$(N-1)N+1$		N^2

$$\rightarrow \quad i = n + (m-1)N \quad \longleftrightarrow \quad (m,n)$$

Eigenvalue Problems

Many physics problems, especially from QM, can be expressed as eigenvalue problems

① $$A\vec{x} = \lambda\vec{x}$$

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1N}x_N = \lambda x_1$$
$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2N}x_N = \lambda x_2$$
$$\vdots$$
$$a_{N1}x_1 + a_{N2}x_2 + \dots + a_{NN}x_N = \lambda x_N$$

like system of linear eq$\underline{n}$s, except RHS is unknown and solutions exist only for certain λ's (eigenvalues)

- solutions are eigenvectors

① can be rewritten as $(A - \lambda I)\vec{x} = 0$

For non-trivial solution $(\vec{x} = 0)$, this implies

$$\det(A - \lambda I) = 0$$

, for which an $N \times N$ matrix leads to an N-degree polynomial for λ

$$c_N\lambda^N + c_{N-1}\lambda^{N-1} + \dots + c_1\lambda + c_0 = 0$$

which has N solutions for λ, i.e., N eigenvalues

Finding all roots for an N-degree polynomial is hard for large N.

Rather than solving the difficult polynomial problem,
iterative methods are used.

e.g. see Jacobi method for symmetric matrices
(which employs "Givens rotations")

or a general method based on QR decomposition.

Let $A_0 = A$

$A_k = Q_k R_k$ Q - orthogonal (bunch of Givens rotations)

R - upper triangular

set
$$
\begin{aligned}
A_{k+1} &= R_k Q_k \\
&= Q_k^{-1} Q_k R_k Q_k \\
&= \underbrace{Q_k^{-1} A_k Q_k}_{\text{similarity transformation}} = Q_k^T A_k Q_k
\end{aligned}
$$

A_k converges to an upper triangular matrix
- eigenvalues of an upper triangular matrix are the diagonals

LAPACK: Different routines for different types of matrices.

Application: Time-Independent Schrödinger Eq$^{\underline{n}}$ in 1-D

ⓘ $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \tilde{V}(x)\psi(x) = \tilde{E}\psi(x)$$

multiply by $\frac{2m}{\hbar^2}$, define $V = \frac{2m}{\hbar^2}\tilde{V}$

$E = \frac{2m}{\hbar^2}\tilde{E}$

discretize: $$\frac{d^2\psi}{dx^2} \rightarrow \frac{\psi_{j-1} - 2\psi_j + \psi_{j+1}}{\Delta x^2}$$

ⓘ becomes $-\psi_{j-1} + (2 + \Delta x^2 V_j)\psi_j - \psi_{j+1} = \Delta x^2 E \psi_j$

If $\psi(x) = 0$ on boundaries, get tridiagonal matrix

$$\begin{pmatrix} 2+V_1\Delta x^2 & -1 & 0 & 0 & \cdots \\ -1 & 2+V_2\Delta x^2 & -1 & 0 & \\ 0 & -1 & 2+V_3\Delta x^2 & -1 & \\ 0 & 0 & -1 & \ddots & \\ & \vdots & & & \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \vdots \end{pmatrix} = \epsilon \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \vdots \end{pmatrix}$$

$$E = \frac{\epsilon}{(\Delta x)^2} \rightarrow \text{eigenvalue}$$

Each eigenvalue will have an associated eigenvector $\vec{\psi}$, the components of which are $\psi(x_i)$ - the eigenfunction sampled at discrete points.

Notes on A4 Q2 show code for A4 Q2

For harmonic potential

1) $V(x) = \frac{1}{2} m \omega^2 x^2$, energy eigenvalues are

2) $E_n = \hbar\omega(n - 1/2)$, $n = 1, 2, \ldots$

Here

$\hbar = 1$, $m = 1/2$

so $V(x) = \frac{1}{4}\omega^2 x^2$

$E_n = \omega(n - 1/2)$

Now,

$V(x) = 10^5 (x - 1/2)^2$

ω: $10^5 = \frac{1}{4}\omega^2$

$\omega = \sqrt{4 \times 10^5}$

$\downarrow$

E: $E_n = \omega(n - 1/2)$

For 3D problems, having N^3 gridpoints makes the problem difficult.

Alternative: write wavefunctions as a linear combination of basis function

$$\psi(\vec{r}) = \sum_\beta a_\beta \phi_\beta(\vec{r})$$

The $\phi_\beta(\vec{r})$'s are known functions that solve part of the problem. E.g. atomic wavefunctions when $\psi(\vec{r})$ is for a molecule.

Goal is to find coefficients a_β that solve the S.E.

$$-\nabla^2\psi + V(\vec{r})\psi = E\psi$$

$$\sum_\beta a_\beta \left(-\nabla^2 + V(\vec{r})\right)\phi_\beta(\vec{r}) = E \sum_\beta a_\beta \phi_\beta(\vec{r})$$

multiply by ϕ_α^* and integrate

$$\sum_\beta \int d^3\vec{r}\, \phi_\alpha^*(\vec{r}) \left(-\nabla^2 + V(\vec{r})\right) \phi_\beta(\vec{r})\, a_\beta$$

$$= E \sum_\beta \int d^3\vec{r}\, \phi_\alpha^*(\vec{r}) \phi_\beta(\vec{r})\, a_\beta$$

Define elements of two matrices

$$H_{\alpha\beta} = \int d^3\vec{r}\, \phi_\alpha^* \left(-\nabla^2 + V(\vec{r})\right) \phi_\beta(\vec{r})$$

$$S_{\alpha\beta} = \int d^3\vec{r}\, \phi_\alpha^*(\vec{r}) \phi_\beta(\vec{r}) \quad \text{(overlap matrix)}$$

Schrödinger Equation becomes

$$\sum_\beta H_{\alpha\beta}\, a_\beta = E \sum_\beta S_{\alpha\beta}\, a_\beta$$

or ✭ $H\vec{a} = E S \vec{a}$ - generalized eigenvalue problem

If ϕ's are orthonormal, then $S = I$ and we get

$$H\vec{a} = E\vec{a}$$

If not, need to transform ✭, as through a Cholesky factorization, an LU decomposition of a positive-definite Hermitian matrix S :

$$S = \underset{\text{lower triangular}}{L}\ \underset{\text{upper triangular}}{L^+} \qquad (L^+_{ij} = L^*_{ji})$$

✭ becomes

$$H I \vec{a} = E L L^+ a$$

$$H (L^+)^{-1} L^+ \vec{a} = E L (L^+\vec{a})$$

$$\underbrace{L^{-1} H (L^+)^{-1}}_{A} \underbrace{(L^+\vec{a})}_{\vec{y}} = E (L^+\vec{a})$$

$$A \quad \vec{y} = E\,\vec{y}$$ – a regular eigenvalue problem

$$\vec{y} = L^+\vec{a}$$

$$\vec{a} = (L^+)^{-1}\vec{y}$$ – eigenvector of original ✭