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

V is electrostatic potential associated with

or gravitational potential with

Discretize second derivative and get

$h =$, $f_n =$, $n =$

$x_0 <$

and we assume that we know

$V_0 =$

$V_{N+1} =$

We get

$n=1$

$n=2$

$n=3$

$\vdots$

$n=N$

which is a matrix equation

$$\begin{pmatrix} \\ \\ \\ \\ \end{pmatrix} \begin{pmatrix} \\ \\ \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \\ \\ \\ \end{pmatrix}$$

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

with A a .

Best to find routine specialized for tridiagonal matrices

→ avoid

→

Show A4, Q1

Show code for Poisson problem

Note: In 2D we have

Can map matrix of unknowns ( ) to a

$(m,n) =$

$i =$

→ $i =$

Eigenvalue Problems

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

(1)

$$a_{11} x_1 + a_{12} x_2 + \dots + a_{1N} x_N = \lambda x_1$$

like system of linear eq$^{\underline{n}}$s, except

and solutions exist only for

- solutions are

(1) can be rewritten as

For non-trivial solution ( ), this implies

, for which an $N \times N$

matrix leads to an

which has N solutions for λ, i.e.,

Finding all roots for an N-degree polynomial

Rather than solving the difficult polynomial problem,

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

or a general method based on QR decomposition.

Let $A_0 =$

$A_k =$ $Q -$

$R -$ upper triangular

set $A_{k+1} =$

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

LAPACK: Different routines for different types of matrices.

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

①

multiply by , define $V =$

$E =$

discretize: $\frac{d^2 \psi}{dx^2} \rightarrow$

① becomes

If $\psi(x) =$, get

$$\begin{pmatrix} \\ \\ \\ \end{pmatrix} \begin{pmatrix} \\ \\ \\ \end{pmatrix} = \epsilon \begin{pmatrix} \\ \\ \\ \end{pmatrix}$$

$E =$

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) $E_n = \hbar \omega (n - \frac{1}{2})$, $n = 1, 2, \ldots$

Here

$\hbar =$, $m =$

so $V(x) =$

$E_n =$

Now,

$V(x) =$

ω:

E:

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

Alternative: write wavefunctions as a linear combination of

$$\psi(\vec{r}) =$$

The $\phi_\beta(\vec{r})$'s are known functions that solve part of the problem. E.g.

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

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

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

$$H_{\alpha\beta} = \int d^3\vec{r}$$

$$S_{\alpha\beta} = \int d^3\vec{r} \qquad \text{(overlap matrix)}$$

Schrödinger Equation becomes

$$\sum_{\beta} \qquad = E \sum_{\beta}$$

or ★ $\qquad = \qquad$ - generalized eigenvalue problem

If ϕ's are orthonormal, then $\qquad$ and we get

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

$$S = L\, L^{+} \qquad (L^{+}_{ij} = L^{*}_{ji})$$

lower triangular $\quad$ upper triangular

★ becomes

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

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

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