Lecture 17

Example: Quantum mechanics

• wave function and Schrodinger equation
• discretization
• preservation of probability
• eigenvalues & eigenstates
• example
Quantum mechanics

- single particle in interval $[0, 1]$, mass $m$

- potential $V : [0, 1] \rightarrow \mathbb{R}$

$\Psi : [0, 1] \times \mathbb{R}_+ \rightarrow \mathbb{C}$ is (complex-valued) wave function

**interpretation:** $|\Psi(x, t)|^2$ is probability density of particle at position $x$, time $t$

(so $\int_0^1 |\Psi(x, t)|^2 \, dx = 1$ for all $t$)

evolution of $\Psi$ governed by *Schroedinger* equation:

$$i\hbar \dot{\Psi} = \left( V - \frac{\hbar^2}{2m} \nabla_x^2 \right) \Psi = H \Psi$$

where $H$ is *Hamiltonian* operator, $i = \sqrt{-1}$
Discretization

let’s discretize position $x$ into $N$ discrete points, $k/N, k = 1, \ldots, N$

wave function is approximated as vector $\Psi(t) \in \mathbb{C}^N$

$\nabla^2$ operator is approximated as matrix

$$\nabla^2 = N^2 \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots & \end{bmatrix}$$

so $w = \nabla^2 v$ means

$$w_k = \frac{(v_{k+1} - v_k)/(1/N) - (v_k - v_{k-1})(1/N)}{1/N}$$

(which approximates $w = \partial^2 v / \partial x^2$)

Example: Quantum mechanics
discretized Schrodinger equation is (complex) linear dynamical system

$$\dot{\Psi} = (-i/\hbar)(V - (\hbar/2m)\nabla^2)\Psi = (-i/\hbar)H\Psi$$

where $V$ is a diagonal matrix with $V_{kk} = V(k/N)$

hence we analyze using linear dynamical system theory (with complex vectors & matrices):

$$\dot{\Psi} = (-i/\hbar)H\Psi$$

solution of Shrodingier equation: $\Psi(t) = e^{(-i/\hbar)tH}\Psi(0)$

matrix $e^{(-i/\hbar)tH}$ propagates wave function forward in time $t$ seconds (backward if $t < 0$)
Preservation of probability

\[
\frac{d}{dt} \|\Psi\|^2 = \frac{d}{dt} \Psi^* \Psi
= \dot{\Psi}^* \Psi + \Psi^* \dot{\Psi}
= ((-i/\hbar)H\Psi)^* \Psi + \Psi^*((-i/\hbar)H\Psi)
= (i/\hbar)\Psi^* H\Psi + (-i/\hbar)\Psi^* H\Psi
= 0
\]

(using \( H = H^T \in \mathbb{R}^{N \times N} \))

hence, \( \|\Psi(t)\|^2 \) is constant; our discretization preserves probability exactly
\[ U = e^{-(i/\hbar)tH} \text{ is unitary, meaning } U^*U = I \]

unitary is extension of \textit{orthogonal} for complex matrix: if \( U \in \mathbb{C}^{N \times N} \) is unitary and \( z \in \mathbb{C}^N \), then

\[
\|Uz\|^2 = (Uz)^*(Uz) = z^*U^*Uz = z^*z = \|z\|^2
\]
Eigenvalues & eigenstates

\( H \) is symmetric, so

- its eigenvalues \( \lambda_1, \ldots, \lambda_N \) are real (\( \lambda_1 \leq \cdots \leq \lambda_N \))
- its eigenvectors \( v_1, \ldots, v_N \) can be chosen to be orthogonal (and real)

from \( Hv = \lambda v \iff (-i/\hbar) Hv = (-i/\hbar) \lambda v \) we see:

- eigenvectors of \( (-i/\hbar)H \) are same as eigenvectors of \( H \), i.e., \( v_1, \ldots, v_N \)
- eigenvalues of \( (-i/\hbar)H \) are \((-i/\hbar)\lambda_1, \ldots, (-i/\hbar)\lambda_N\) (which are pure imaginary)

Example: Quantum mechanics
• eigenvectors \( v_k \) are called \textit{eigenstates} of system

• eigenvalue \( \lambda_k \) is \textit{energy} of eigenstate \( v_k \)

• for mode \( \Psi(t) = e^{-i\frac{\hbar}{\hbar} \lambda_k t} v_k \), probability density

\[
|\Psi_m(t)|^2 = |e^{-i\frac{\hbar}{\hbar} \lambda_k t} v_k|^2 = |v_{mk}|^2
\]

doesn’t change with time (\( v_{mk} \) is \( m \)th entry of \( v_k \))
Example
Potential Function $V(x)$

- potential bump in middle of infinite potential well
- (for this example, we set $\hbar = 1$, $m = 1 \ldots$)
lowest energy eigenfunctions

- potential $V$ shown as dotted line (scaled to fit plot)
- four eigenstates with lowest energy shown (i.e., $v_1, v_2, v_3, v_4$)
now let’s look at a trajectory of $\Psi$, with initial wave function $\Psi(0)$

- particle near $x = 0.2$
- with momentum to right (can’t see in plot of $|\Psi|^2$)
- (expected) kinetic energy half potential bump height
- top plot shows initial probability density $|\Psi(0)|^2$
- bottom plot shows $|v_k^*\Psi(0)|^2$, i.e., resolution of $\Psi(0)$ into eigenstates

Example: Quantum mechanics
time evolution, for $t = 0, 40, 80, \ldots, 320$:

$|\Psi(t)|^2$
cf. classical solution:

- particle rolls half way up potential bump, stops, then rolls back down

- reverses velocity when it hits the wall at left (perfectly elastic collision)

- then repeats
plot shows probability that particle is in left half of well, i.e., \[ \sum_{k=1}^{N/2} |\Psi_k(t)|^2, \]
versus time \( t \)

Example: Quantum mechanics