UNIVERSITY OF TEXAS ARLINGTON

PHYS 5319-001: Math Methods in Physics III

Gram-Schmidt orthonormalization

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A technical to get the eigenstate of a given Hamiltonian

$$H\varphi_n = E_n\varphi_n$$

e^{-x}

- If we don't now the eigenstates of *H*, we can start with a trial wavefunction (normalized), $\tilde{\psi}(x,0)$.
- Apply on it repeatedly, each time normalized. $\tilde{a}_0$will grow.
- Eventually we'll get the ground state: $\tilde{\psi}(x,0) \rightarrow \varphi_0$

Start with a trial wavefunction (could be random)

$$\tilde{\psi}(x,0) = \sum_n a_n \varphi_n(x)$$

$E_0 < E_1 < E_2 \ldots$

$$\psi(x,\Delta t) = e^{-\frac{\hat{H}\Delta t}{\hbar}}\psi(x,0) = \sum_n \underline{a_n e^{\frac{-E_n \Delta t}{\hbar}}}\varphi_n(x) \quad = \sum_n \underline{\tilde{a}_n}\varphi_n(x)$$

Normalized this function

In the new set of $\{\tilde{a}_n = a_n e^{\frac{-E_n\Delta t}{\hbar}}\}$, the weight in lowest states is higher.

If we repeat $\psi(x, 2\Delta t) = e^{-\frac{\hat{H}\Delta t}{\hbar}}\psi(x,\Delta t)$ and normalize many, many times

$$\tilde{\psi}(x, \Delta t \rightarrow \infty) \rightarrow \varphi_0(x)$$

How to find the lowest *m* eigenstates?

THEOREM 5.12 Gram-Schmidt Orthonormalization Process

1. Let $B = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ be a basis for an inner product space V.
2. Let $B' = \{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_n\}$, where

$\langle w_1, w_2 \rangle = \langle w_1, v_2 \rangle - \langle v_1, w_1 \rangle$
$= 0$

$$\mathbf{w}_1 = \mathbf{v}_1$$

$$\mathbf{w}_2 = \mathbf{v}_2 - \frac{\langle \mathbf{v}_2, \mathbf{w}_1 \rangle}{\langle \mathbf{w}_1, \mathbf{w}_1 \rangle}\mathbf{w}_1$$

$$\mathbf{w}_3 = \mathbf{v}_3 - \frac{\langle \mathbf{v}_3, \mathbf{w}_1 \rangle}{\langle \mathbf{w}_1, \mathbf{w}_1 \rangle}\mathbf{w}_1 - \frac{\langle \mathbf{v}_3, \mathbf{w}_2 \rangle}{\langle \mathbf{w}_2, \mathbf{w}_2 \rangle}\mathbf{w}_2$$

$$\vdots$$

$$\mathbf{w}_n = \mathbf{v}_n - \frac{\langle \mathbf{v}_n, \mathbf{w}_1 \rangle}{\langle \mathbf{w}_1, \mathbf{w}_1 \rangle}\mathbf{w}_1 - \frac{\langle \mathbf{v}_n, \mathbf{w}_2 \rangle}{\langle \mathbf{w}_2, \mathbf{w}_2 \rangle}\mathbf{w}_2 - \cdots - \frac{\langle \mathbf{v}_n, \mathbf{w}_{n-1} \rangle}{\langle \mathbf{w}_{n-1}, \mathbf{w}_{n-1} \rangle}\mathbf{w}_{n-1}.$$

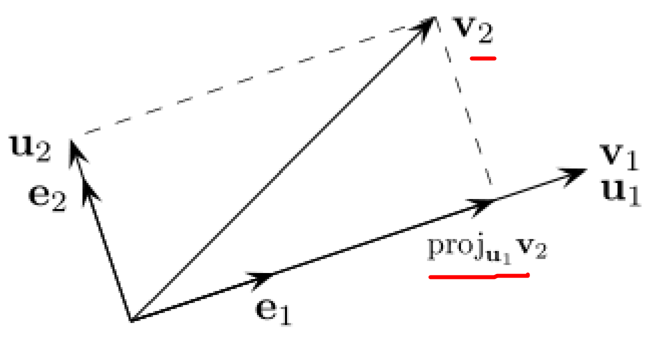
Then B' is an *orthogonal* basis for V.

3. Let $\mathbf{u}_i = \dfrac{\mathbf{w}_i}{\|\mathbf{w}_i\|}$. Then $B'' = \{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n\}$ is an *orthonormal* basis for V.

Also, $\operatorname{span}\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k\} = \operatorname{span}\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_k\}$ for $k = 1, 2, \ldots, n$.

Gram-Schmidt Orthogonalization

- Crucial to carrying out the expansions and transformations under discussion is the availability of useful orthonormal sets of functions.



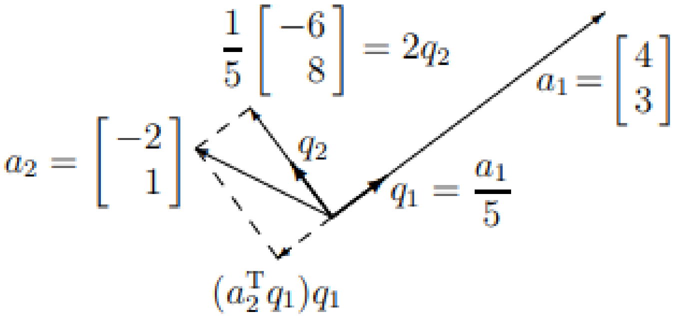
EXAMPLE A is 2 by 2. The columns of Q, normalized by $\frac{1}{5}$, are q_1 and q_2:

$$A = \begin{bmatrix} 4 & -2 \\ 3 & 1 \end{bmatrix} = \frac{1}{5}\begin{bmatrix} 4 & -3 \\ 3 & 4 \end{bmatrix}\begin{bmatrix} 5 & -1 \\ 0 & 2 \end{bmatrix} = QR\,.$$

Starting with the columns a_1 and a_2 of A, Gram-Schmidt normalizes a_1 to q_1 and subtracts from a_2 its projection in the direction of q_1. Here are the steps to the q's:

$$a_1 = \begin{bmatrix} 4 \\ 3 \end{bmatrix} \quad q_1 = \frac{1}{5}\begin{bmatrix} 4 \\ 3 \end{bmatrix} \quad a_2 = \begin{bmatrix} -2 \\ 1 \end{bmatrix} \quad v = a_2 - (q_1^{\mathrm{T}} a_2) q_1 = \frac{1}{5}\begin{bmatrix} -6 \\ 8 \end{bmatrix} \quad q_2 = \frac{1}{5}\begin{bmatrix} -3 \\ 4 \end{bmatrix}$$

Along the way, we divided by $\|a_1\| = 5$ and $\|v\| = 2$. Then 5 and 2 go on the diagonal of R, and $q_1^{\mathrm{T}} a_2 = -1$ is $R(1,2)$. This figure shows every vector:



To implement

- In: $\{\boldsymbol{v}_i\}$, n-din×m array
- Out: $\{\boldsymbol{w}_i\}$, orthonormalized vector set
- Use scalar product function (LAPACK) SDOT()

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REAL FUNCTION SDOT ( n, x, incx, y, incy )
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$\langle x|y\rangle$

- Start Gram-Schdmit

w_1=v_1

Loop *i=2,m*

$$w_i = v_i - \frac{\langle v_i|w_1\rangle}{\langle w_1|w_1\rangle} w_1 - \frac{\langle v_i|w_2\rangle}{\langle w_2|w_2\rangle} w_2 - \cdots - \frac{\langle v_i|w_{i-1}\rangle}{\langle w_{i-1}|w_{i-1}\rangle} w_{i-1}$$

end loop

normalize $\{\boldsymbol{w}_i\}$

Gram-Schmidt in 9 Lines of MATLAB

```
for j=1:n                       % Gram-Schmidt orthogonalization
  v=A(:,j);                     % v begins as column j of A
  for i=1:j-1
    R(i,j)=Q(:,i)'*A(:,j);      % modify A(:,j) to v for more accuracy
    v=v-R(i,j)*Q(:,i);          % subtract the projection (q_i^T a_j)q_i = (q_i^T v)q_i
  end                           % v is now perpendicular to all of q_1,...,q_{j-1}
  R(j,j)=norm(v);
  Q(:,j)=v/R(j,j);              % normalize v to be the next unit vector q_j
end
```

Transform any ***A*** to an orthogonal ***A'***

$$\boldsymbol{A} = \boldsymbol{QR} \Rightarrow \boldsymbol{A}' = \boldsymbol{Q}^T\boldsymbol{AQ}$$

In LAPACK, this is subprogram called “dgeqrf()”

$$H\varphi_n = E_n\varphi_n$$

Start with a set of trial wavefunctions (could be random)

$$\tilde{\psi}_i(x,0) = \sum_n a_n^i \varphi_n(x), i = 1,2,..,m$$

$$\psi_i(x,\Delta t) = e^{-\frac{\hat{H}\Delta t}{\hbar}}\psi_i(x,0) = \sum_n a_n^i e^{\frac{-E_n\Delta t}{\hbar}}\varphi_n(x) = \sum_n \tilde{a}_n^i \varphi_n(x)$$

Apply Gram-Schmidt scheme to {$\psi_i(x,\Delta t)$}

If we repeat $\psi_i(x,2\Delta t) = e^{-\frac{\hat{H}\Delta t}{\hbar}}\psi_i(x,\Delta t)$ and orthonormalize many, many times

$$\widetilde{\psi_1}(x,\Delta t \to \infty) \to \varphi_0(x)$$
$$\widetilde{\psi_2}(x,\Delta t \to \infty) \to \varphi_1(x)$$
$$\dots \dots$$

Now, how to calculate $\psi_i(x,\Delta t) = e^{-\frac{\hat{H}\Delta t}{\hbar}}\psi_i(x,0)$?

For small Δt (also assuming $\hbar$=1, m=1), we take Taylor expansion: $e^{-\hat{H}\Delta t} \approx 1 - \hat{H}\Delta t$

Error $\sim O(\Delta t^2)$

$$\psi_i(x,\Delta t) = e^{-\hat{H}\Delta t}\psi_i(x,0) \approx \left(1 - \hat{H}\Delta t\right)\psi_i(x,0)$$

Still, $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) = -\frac{1}{2}\frac{d^2}{dx^2} + V(x)$.

How to evaluate $\left[-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right] f(x)$?

$V(x)\,f(x)$ is easy (on grid)

Do $\left(-\frac{1}{2}\frac{d^2}{dx^2}\right) f(x)$ in Fourier space: FFT $f(x_n) \to g(k_n) \to \frac{1}{2}k_n^2 g(k_n) \to FFT^{-1}$back

Add the 2 terms in x-space

We have N discrete k-points:

$$k_n = \frac{2\pi n}{L}, n = 0, 1, 2, \ldots, N-1$$

Or $n = -\frac{N}{2}, -\frac{N}{2}+1, \ldots, 0, 1, \ldots \frac{N}{2}-1$

Convergence check?

Calculate the expectation values:

$$\langle E_i \rangle = \langle \psi_i | H | \psi_i \rangle$$

Iterations until converged, $|\Delta E_i| < \varepsilon \;\; (e.g. 10^{-5})$

Save $\{\psi_i\}, \{E_i\}$ $to\ disk$

Run could be continued