Computational Physics

⊙ What problems in Physics can one solve with a computer ?

Gravitational problems → ODEs PDEs ← (4)

Navier – Stokes

Electromagnetism

Kinetic theory

MINIMIZATION of function of many variables (3)

Minimization problems : energy minimization

Search of fixed points

(Fast Fourier transform / signal analysis)

Eigenvalue problems (1) ex: (quantum mechanics)

Calculation of multi-dimensional integrals (2)

Computational problems : scaling of computing time

" Size of the problem " : $\underline{N}$ # of degrees of freedom

(D dimensions of the problem)

$\underline{\epsilon}$: accuracy of the solution

$T(N, \epsilon)$?

time to solution

Efficient algorithm

$\alpha < \infty$

$$T(N, \epsilon) \sim \begin{cases} \text{poly}_{\underline{n}}(N) & (\text{ex. } \sim N^4.) \\ \text{poly}_n\left(\frac{1}{\epsilon}\right) & \left(\sim \left(\frac{1}{\epsilon}\right)^n\right) \end{cases}$$

Inefficient algorithm / hard computational problem

$$T(N, \underline{\epsilon}) \sim \begin{cases} B \cdot \exp(A N^{\alpha}) \\ B \exp\left(A \frac{1}{\epsilon^{\alpha}}\right) \end{cases}$$

Eigenvalue problems

A Hermitian $N \times N$ matrix

$A^+ = A \qquad A_{ij} = A^*_{ji} \in \mathbb{C}$

$$\boxed{A \vec{x}_k = \lambda_k \vec{x}_k} \qquad k = 1, \dots, N$$

$$\rightsquigarrow \left(A | x_k \rangle = \lambda_k | x_k \rangle \right)$$

$\lambda_k \in \mathbb{R}$

1) Quantum mechanics

$$\hat{O} | \psi_k \rangle = O_k | \psi_k \rangle \qquad | \psi \rangle \in H$$

$\left(\begin{array}{l} O_k \in \mathbb{R} \\ \hat{O} = \hat{O}^+ \end{array} \right)$

basis of Hilbert space H

$\{ | \phi_n \rangle \}$ $\qquad n = 1, \dots, D$

$$\sum_{n=1}^{D} | \phi_n \rangle \langle \phi_n | = \mathbb{1}_D$$

$$\left(\sum_n \vec{\phi}_n \vec{\phi}_n^T = \mathbb{1} \right)$$

$\langle \phi_m |$ $\qquad \langle \phi_m |$

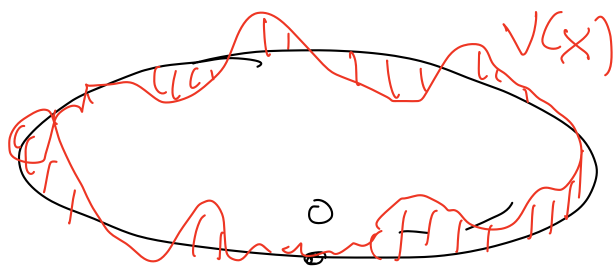
$$\sum_n \hat{O} | \phi_n \rangle \langle \phi_n | \psi_k \rangle = O_k | \psi_k \rangle$$

$$\boxed{\sum_n O_{mn}\,\psi_n^{(k)} = o_k\,\psi_m^{(k)}}$$

$$\underbrace{\langle \phi_m | \hat{O} | \phi_n \rangle = O_{mn}}$$

$$\langle \phi_m | \psi_k \rangle = \psi_m^{(k)}$$

<u>Example</u> : 1d particle in a potential (with periodic boundary conditions)



$x = 0 \equiv L$

$L =$ length of the ring

$$\hat{H} = \frac{\hat{p}^2}{2M} + V(\hat{x})$$

a) momentum basis

$|q_n\rangle$: $\hat{p}|q_n\rangle = \hbar q_n |q_n\rangle$

$$\langle x | q_n \rangle = \frac{1}{\sqrt{L}} e^{i q_n x} \qquad q_n = \frac{2\pi}{L} n$$

$n \in \mathbb{Z}$

truncate the dimensions of H from ∞ to D

n : $-\frac{D}{2}+1, \ldots, \frac{D}{2}$

$$\langle q_n|\mathcal{H}|q_m\rangle = \frac{\hbar^2 q_n^2}{2M}\,\delta_{nm} \leftarrow$$

$$+ \underbrace{\langle q_n|\,V(\hat{x})\,|q_m\rangle}$$

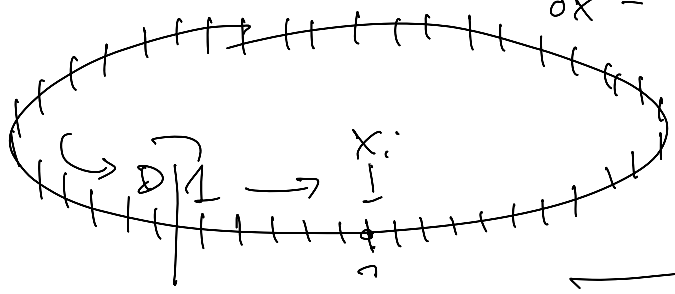
(ex.) $$\frac{1}{L}\int dx\; V(x)\; e^{-i(q_n-q_m)x}$$

$$\begin{pmatrix} \frac{\hbar^2 q_1^2}{2M} + \langle q_1|V|q_1\rangle & \langle q_1|V|q_2\rangle & \cdots \\ \langle q_2|V|q_1\rangle & \frac{\hbar^2 q_2^2}{2M} + \langle q_2|V|q_2\rangle & \cdots \\ \vdots & & \ddots \end{pmatrix}$$

$$|q_n| < \frac{2\pi}{L}D \qquad\qquad \underline{\delta x > \frac{L}{D} = (\delta x)_{min}}$$

b) discretized position basis $|x\rangle$

$$\delta x = \frac{L}{D} \qquad x \in [0, L]$$



$$\langle x|\hat{\mathcal{H}}|\psi\rangle = \langle x|E|\psi\rangle \to \left(-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\,\psi(x)$$

$$\frac{d}{dx}\psi(x)\Big|_{x=x_i} = \frac{\psi(x_{i+1})-\psi(x_i)}{\delta x} + o(\delta x)$$

$x_i + \delta x$

$$\frac{d^2}{dx^2}\psi(x)\Big|_{x_i} \approx \frac{\psi(x_{i+1})+\psi(x_{i-1})-2\psi(x_i)}{(\delta x)^2} + o(\delta x)$$

$V(x_i) = V_i$

$\psi(x_i) \Rightarrow \psi_i$

ϵ_0

$$\boxed{-\frac{\hbar^2}{2M(\delta x)^2}\left(\psi_{i+1}+\psi_{i-1}-2\psi_i\right) + V_i\psi_i = E\psi_i}$$

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

$$H = \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & \cdots & D \end{array} \\ \begin{pmatrix} V_1+2\epsilon_0 & -\epsilon_0 & & & -\epsilon_0 \\ -\epsilon_0 & V_2+2\epsilon_0 & -\epsilon_0 & & \\ & -\epsilon_0 & \ddots & \ddots & \\ & 0 & \ddots & \ddots & \\ -\epsilon_0 & & & & V_D+2\epsilon_0 \end{pmatrix} \end{array}$$

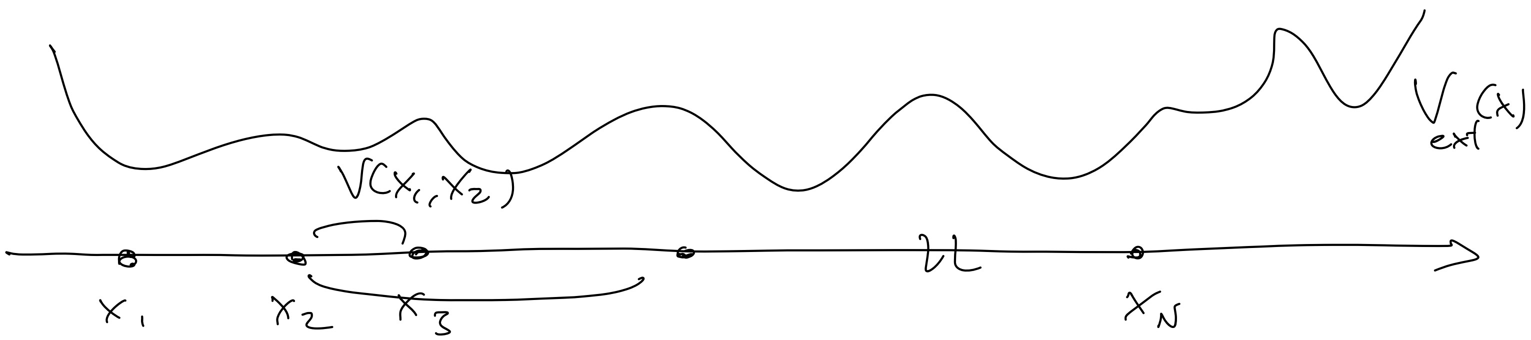
$N + (N-1)2$

$+2$

$= 2N$

sparse matrix

2) Normal-mode analysis



$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2M} + \underbrace{\sum_i V_{ext}(x_i) + \frac{1}{2}\sum_{i \neq j} V(x_i, x_j)}_{U(\{x_i\})}$$

$$M \ddot{x}_k = -\frac{\partial}{\partial x_k} U$$

$$\underline{\min\ U(\{x_i\})} \Rightarrow x_i = x_i^{(0)}$$

$$U(\{x_i\}) = U(\{x_i^{(0)}\}) + \sum_{i=1}^{N} \cancel{\left(\frac{\partial}{\partial x_i} U \Big|_{\{x_i^{(0)}\}}\right)} (x_i - x_i^{(0)})$$

$$+ \frac{1}{2} \sum_{i,j} \underbrace{\frac{\partial^2 U}{\partial x_i \partial x_j}\Big|_{\{x_i^{(0)}\}}}_{H_{ij}} (x_i - x_i^{(0)})(x_j - x_j^{(0)}) + \ldots$$

$$0$$

Hessian

$$M\ddot{x}_k = -\sum_j H_{kj}\left(x_j - x_j^{(0)}\right)$$

$$\longrightarrow \quad y_k = x_k - x_k^{(0)}$$

$$\tilde{H}_{kj}$$

$$\ddot{y}_k = -\sum_j \frac{H_{kj}}{M}\, y_j \qquad k = 1, \to N$$

$$\boxed{\ddot{\vec{y}} = -\tilde{H}\,\vec{y}}$$

$$\vec{y}(t) = \vec{y}(0)\, e^{i(\omega t + \phi)}$$

$$\hookrightarrow \cos(\omega t + \phi)$$

$$\omega_n^2\, \vec{y}_n(0) = \tilde{H}\,\vec{y}_n(0)$$

diagonalize the Hessian matrix

$\tilde{H}$: semi-positive definite

$$\Rightarrow \quad \omega^2 \geq 0$$

$U_{ext} = 0$ $\qquad \vec{y}_n = \{\cos(q_n x_n)\}$

Full diagonalization of a matrix

LAPACK

QR algorithm

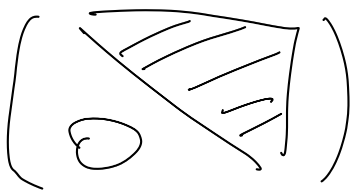
$$\boxed{O(N^3)}$$

$A = QR$ → upper triangular matrix

Hermitian $\quad$ ↓

$N \times N$ $\quad$ unitary

$Q^\dagger Q = \mathbb{1}$



$$A_1 = RQ = Q^\dagger A Q = Q_1 R_1$$

$$A_2 = R_1 Q_1 = Q_1^\dagger A_1 Q_1 = Q_2 R_2$$

$$\ldots$$

A_k diagonal $\qquad k \gg 1$

Storage :

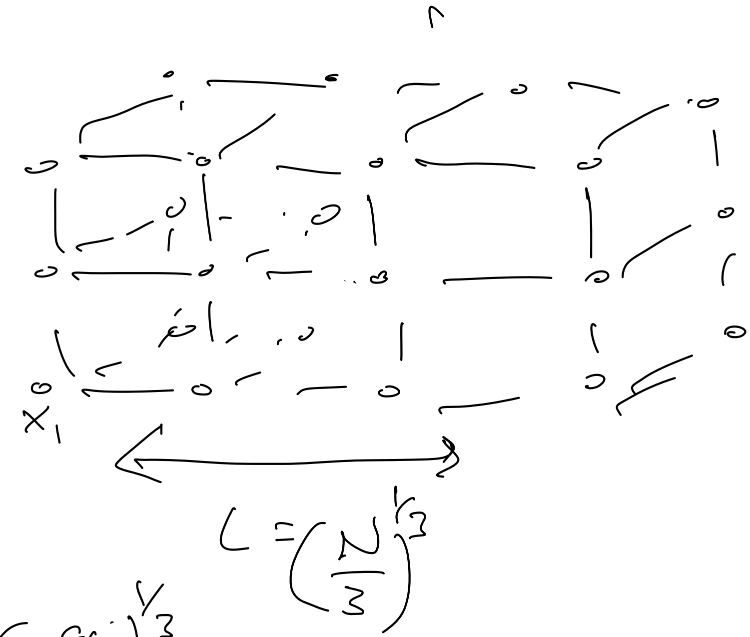
N^2 matrix elements

8 bytes for each number

RAM $\quad n \times 10^9$ bytes $\qquad n \simeq 10$

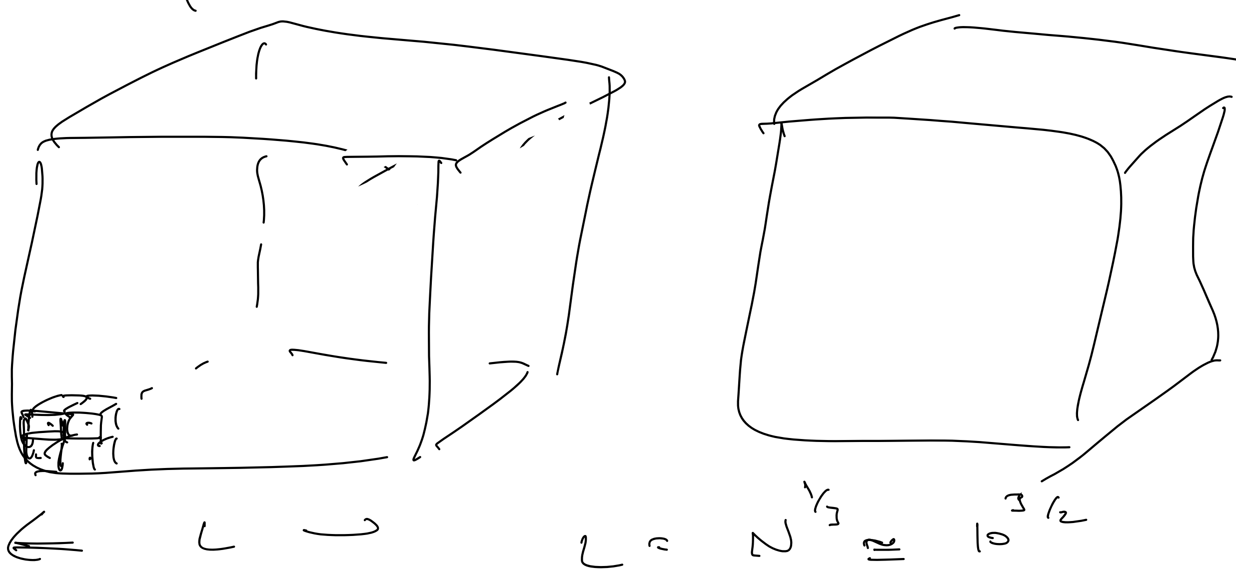
$$N^2 = \frac{\cancel{n} \times 10^9}{\cancel{8}} \simeq 10^9$$

$N = 10^{9/2} \simeq 32000$



$$L = \left(\frac{10^{9/2}}{3}\right)^{1/3} \simeq 22$$

1 quantum particle in 3d



$L = N^{1/3} \simeq 10^{3/2}$

$\simeq 32$

$$L = \sqrt{N^{1/3}} \simeq 6$$

Tricks

② A : $N \times N$ Sparse matrix
\# of non-zero elements being of $O(N^\alpha)$, $\alpha < 2$

⓪ Use symmetries

$$[A, \underline{V}] = 0 = AV - VA$$

A, V admit a common basis of eigenvectors

$\underline{V}$ is easy to diagonalize

$$\Rightarrow V \vec{v}_n^{(k)} = \lambda_k \vec{v}_n^{(k)}$$

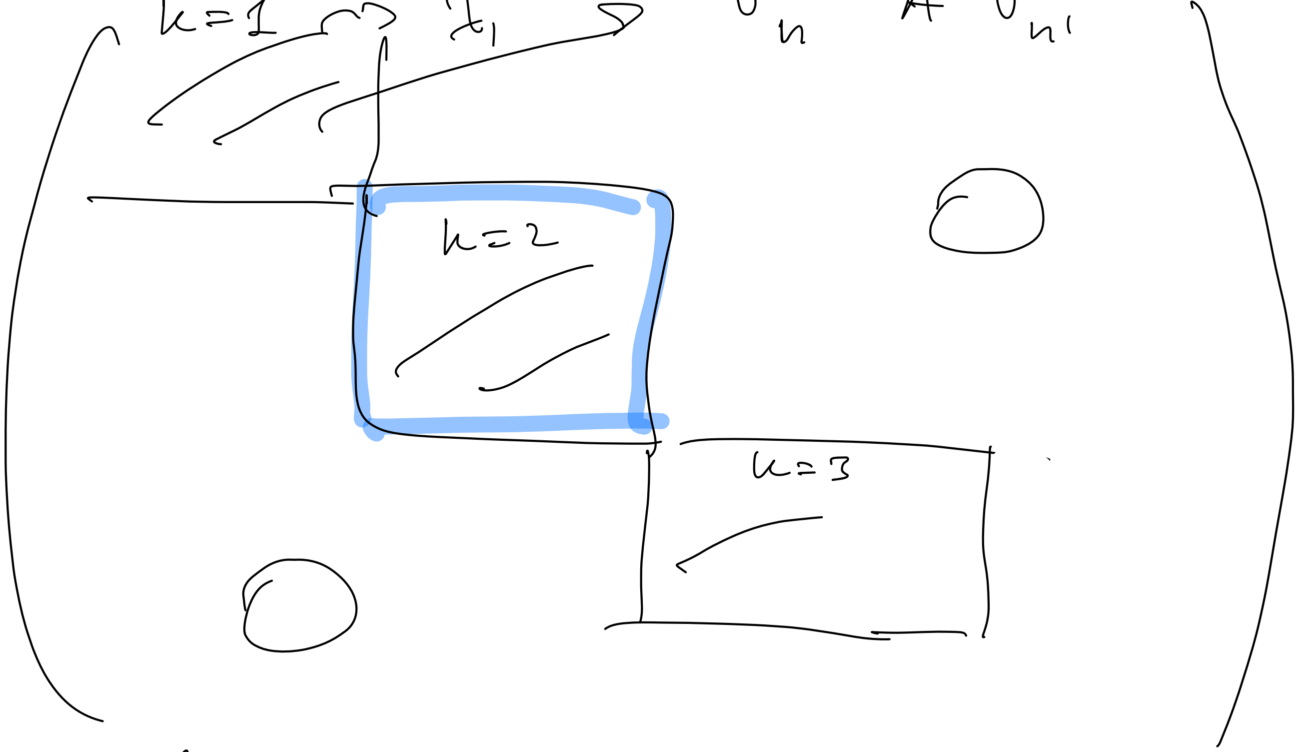
d_k degeneracy of the k-th eigenvalue
$n = 1, \dots, d_k$

within the degenerate eigenspace $\{ v_n^{(k)} \}$ $n = 1, \dots, d_k$
I can find an eigenvector of A

$$\underbrace{\left(\vec{v}_n^{(k)}\right)^T A \, \vec{v}_{n'}^{(k')}} \sim \delta_{kk'}$$

$\vec{v}^{(1)T} A \, \vec{v}^{(1)}$

$=$



{Ex. $A = \hat{H}$ which is translationally invariant
$V = \hat{p}$ momentum operator }.

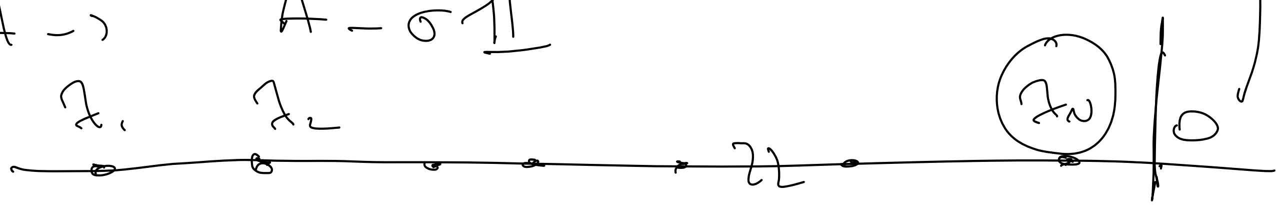
Determination of the <u>extreme eigenvalues</u>

→ power method $\left(A^n \vec{u} \right)$

A : $N \times N$

$$\begin{cases} \lambda_1 < \lambda_2 < \dots < \lambda_N \\ |\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \dots \geq |\lambda_N| \end{cases}$$

$A \to A - \sigma \mathbb{1}$



non degenerate

$$A\vec{v}_1 = \lambda_1 \vec{v}_1$$

$$A\vec{v}_k = \lambda_k \vec{v}_k$$

$\vec{u}$ random vector

$$c_1 = \boxed{\vec{v}_1^{\dagger} \cdot \vec{u} \neq 0}$$

$$A^n \vec{u} = A^n \left(\sum_{k=1}^{N} c_k \vec{v}_k \right)$$

$$= A^n \left(c_1 \vec{v}_1 + \sum_{k=2}^{N} c_k \vec{v}_k \right)$$

$$= c_1 \lambda_1^n \vec{v}_1 + \sum_{k=2}^{N} c_k \lambda_k^n \vec{v}_k$$

$$= \lambda_1^n \left(c_1 \vec{v}_1 + \sum_{k=2}^{N} c_k \left(\frac{\lambda_k}{\lambda_1} \right)^n \vec{v}_k \right)$$

$n \to \infty$ 0

$$\left| \frac{\lambda_k}{\lambda_1} \right| < 1$$

$$\exp\left[- \left| \log \left| \frac{\lambda_k}{\lambda_1} \right| \right| n \right]$$

$$\mathrm{sign}\left(\frac{\lambda_k}{\lambda_1} \right)$$

$$\xrightarrow[n \to \infty]{} \lambda_1^n c_1 \vec{v}_1$$

$$\boxed{\frac{A^{n}\vec{u}}{\|A^{n}\vec{u}\|} \xrightarrow{n\to\infty} \vec{v}_1}$$

convergence is exponential with a rate

$$\Rightarrow \left|\log\left|\frac{\lambda_2}{\lambda_1}\right|\right|$$

$\vec{u}, A\vec{u}, A^{2}\vec{u} = A(A\vec{u}),$

$A^{3}\vec{u}, \ldots, A^{M-1}\vec{u}$

$\underbrace{\qquad\qquad}_{}$ M vectors

$\text{span}(\vec{u}, A\vec{u}, A^{2}\vec{u}, \ldots, A^{M-1}\vec{u}) = K_M$

Krylov space

if $\vec{u}$ is not an eigenvector of A

$\dim(K_M) = M$

Gram-Schmidt orthogonalization

$\vec{u}$'s normalized $\|\vec{u}\| = 1$

$\vec{u}_0 = \vec{u}$ $\|\vec{u}_k\| = 1$

$$\beta_1 \vec{u}_1 = A\vec{u}_0 - \underbrace{(\vec{u}_0^{+} A \vec{u}_0)}_{\alpha_0} \vec{u}_0$$

$$\beta_2 \vec{u}_2 = A\vec{u}_1 - \underbrace{(\vec{u}_1^{+} A \vec{u}_1)}_{\alpha_1} \vec{u}_1 - (\vec{u}_0^{+} A \vec{u}_1)\vec{u}_0$$

$$\beta_3 \vec{u}_3 = A\vec{u}_2 - \underbrace{(\vec{u}_2^{+} A \vec{u}_2)}_{\alpha_2} \vec{u}_2 - (\vec{u}_1^{+} A \vec{u}_2)\vec{u}_1 - \underbrace{(\vec{u}_0^{+} \cancel{A \vec{u}_2})}_{0} \vec{u}_0$$

$$\vec{u}_0^{+} A \vec{u}_2 = (A\vec{u}_0)^{+} \cdot \vec{u}_2$$

$$= \left(\beta_1 \vec{u}_1 + (\vec{u}_0^{+} A \vec{u}_0)\vec{u}_0\right)^{+} \cdot \vec{u}_2 = 0$$

$$\boxed{\beta_k \vec{u}_k = A\vec{u}_{k-1} - (\vec{u}_{k-1}^{+} A \vec{u}_{k-1})\vec{u}_{k-1} - (\vec{u}_{k-2}^{+} A \vec{u}_{k-1})\vec{u}_{k-2}}$$

Lanczos basis $k = M-1$

M vectors

$$\{(\vec{u}_k^{\dagger} A \vec{u}_l)\} = \{\tilde{A}_{kl}\} \qquad M \times M$$

$$= \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & 0 \\ & \beta_2 & \alpha_2 & \beta_3 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & \ddots & \ddots \end{pmatrix}$$

tridiagonal matrix

$\downarrow$

diagonalized in time $\sim \mathcal{O}(N^2)$

$$\alpha_k = \vec{u}_k A \vec{u}_k$$

eigenvalues & eigenvectors of $\tilde{A}$ approximate the first M eig. / eig. of A