Computational Physics

Scaling properties of the algorithm for a problem

- # of degrees of freedom involved by the problem N
- # of dimensions D

(ex. $N \simeq 10^{23}$
$D = 6N$)

- precision of the solution
  $a \pm \varepsilon$

T : time to solution

Scaling : property of an algorithm

Bad scaling : $T \simeq A \exp(N^{\alpha})$
$= A \exp(D^{\alpha})$
$\simeq A \exp\left(\frac{1}{\varepsilon^{\alpha}}\right)$

Good scaling : $T \simeq \mathrm{poly}_n(N)$
$\mathrm{poly}_n(D)$

$\mathrm{poly}_n\left(\frac{1}{\varepsilon}\right)$

exp $\to$ poly

① Large eigenvalue problems

A matrix, square $N \times N$, Hermitian $A = A^\dagger$

$\vec{v}_n \in \mathbb{C}^N$ $A_{ij} = A^*_{ji} \in \mathbb{C}$

$A \vec{v}_n = \lambda_n \vec{v}_n$ $\lambda_n \in \mathbb{R}$

$n = 1, \dots, N$

$U^\dagger A U = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_N) = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & \ddots & \lambda_N \end{pmatrix}$

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

$\vec{x}_n = \frac{\vec{v}_n}{\|\vec{v}_n\|}$

$U = \begin{pmatrix} \vec{x}_1 & \vec{x}_2 & \dots & \vec{x}_N \end{pmatrix}$

1) Quantum mechanics

Abstract problem

observable $\longrightarrow$ $\hat{O}$ operator

on a Hilbert space $\mathcal{H}$

$\dim(\mathcal{H}) = D$

$\vec{\psi}_u$

$$\hat{O}\,|\psi_u\rangle = o_u\,|\psi_u\rangle \qquad o_u \in \mathbb{R}$$

possible measurement results

$\nearrow \mathbb{1}$

Basis of Hilbert space

$\{|\phi_n\rangle\}$ orthonormal vectors $\langle\phi_n|\phi_m\rangle = \delta_{nm}$

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

$\langle\phi_n|$ $\qquad\qquad\qquad\qquad$ $\langle\phi_n|$

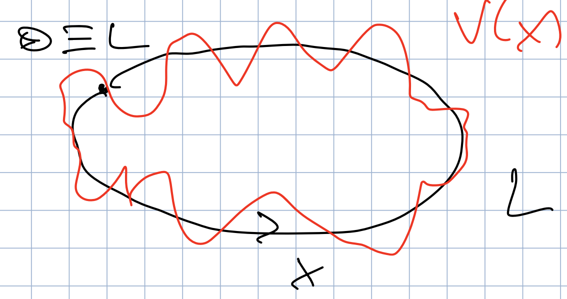
$$\sum_m \hat{O}\,|\phi_m\rangle\langle\phi_m|\psi_u\rangle = o_u\,|\psi_u\rangle$$

$$\sum_m \langle\phi_n|\hat{O}|\phi_m\rangle\,\psi_m^{(u)} = o_u\,\psi_n^{(u)}$$

O_{nm}

$$\overline{O}\,\vec{\psi}^{(u)} = o_u\,\vec{\psi}^{(u)}$$

Example



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

Choose a basis

1) momentum basis

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

$$q_n \equiv \frac{2\pi}{L} n \qquad n \in \mathbb{Z}$$

$$\underbrace{-\infty, \to \infty}_{-\frac{D}{2}+1,\ -\frac{D}{2}+2,\ \dots,\ \frac{D}{2}}$$

D values

$$H_{nm} = \langle q_n | \hat{H} | q_m \rangle$$

$$= \frac{\hbar^2 q_n^2}{2M}\,\delta_{nm} + \overbrace{\langle q_n | V(\hat{x}) | q_m \rangle}^{V_{nm}}$$

$$\int dx \; |x\rangle\langle x| = \mathbb{1} \qquad \frac{1}{\sqrt{L}} e^{i q_m x} \qquad \boxed{\hat{x}|x\rangle = x|x\rangle}$$

$$\Longrightarrow$$

$$\int dx \; \langle q_n | x\rangle \langle x | q_m\rangle V(x)$$

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

$$\tilde{V}(q_m - q_n)$$

$$\left(-\frac{D}{2}+1\right)\frac{2\pi}{L} \leq q_n \leq \frac{D}{2}\frac{2\pi}{L} \qquad |q_n - q_m| \leq \frac{2\pi}{L} D$$

$$= \frac{2\pi}{\lambda}$$

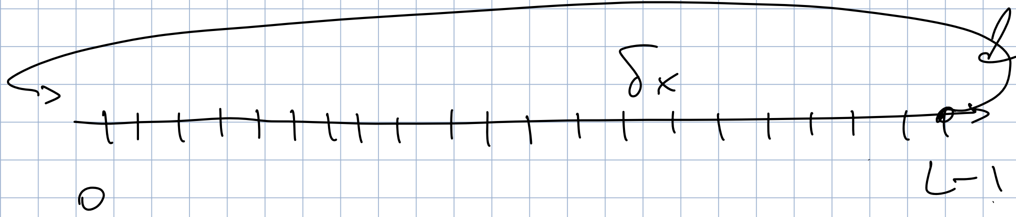
$$\boxed{\lambda \geq \frac{L}{D}}$$

$$\{H_{nm}\} = \begin{pmatrix} \frac{\hbar^2 q_1^2}{2M} + \frac{\tilde{V}(0)}{L} & V_{12} & V_{13} \\ V_{21} & \frac{\hbar^2 q_2^2}{2M} + \frac{\tilde{V}(0)}{L} & \\ & & \ddots \end{pmatrix}$$

2) <u>position basis</u>

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$\left(-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\,\psi(x)$$



$$D = \frac{L}{\delta x}$$

$$|x\rangle \to |x_i\rangle \qquad x_i = (i-1)\,\delta x$$

$$\psi(x) \to \psi(x_i)$$

$$V(x) \to V(x_i) \qquad x_{i+1} = x_i + \delta x$$

$$\left.\frac{d\psi}{dx}\right|_{x_i} \simeq \frac{\psi(x_{i+1}) - \psi(x_i)}{\delta x} + O(\delta x)$$

$$\left.\frac{d^2\psi}{dx^2}\right|_{x_i} = \frac{\psi(x_{i+1}) + \psi(x_{i-1}) - 2\psi(x_i)}{(\delta x)^2} + O(\delta x)$$

$$-\overset{\epsilon_0}{\frac{\hbar^2}{2M(\delta x)^2}}\left[\psi(x_{i+1}) + \psi(x_{i-1})\right] + \overset{\epsilon_0}{\frac{\hbar^2}{2M(\delta x)^2}}\,2\psi(x_i)$$

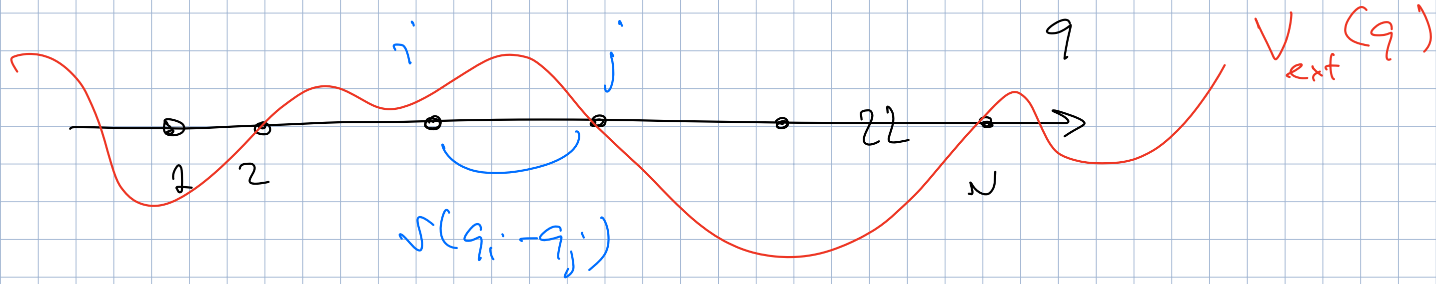
$$+ V(x_i)\,\psi(x_i) = E\,\psi(x_i)$$

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

$$\{\tilde{H}_{ij}\} = \begin{array}{c} \begin{array}{ccccc} 1 & & & & D \end{array} \\ \begin{pmatrix} V(x_1)+2\epsilon_0 & -\epsilon_0 & & 0 & -\epsilon_0 \\ -\epsilon_0 & V(x_2)+2\epsilon_0 & -\epsilon_0 & & \\ & -\epsilon_0 & \ddots & & \\ 0 & & & \ddots & \\ -\epsilon_0 & & & & V(x_D)+2\epsilon_0 \end{pmatrix} \end{array}$$

2) Classical physics : Linearization of Newton's equation (normal-mode analysis)

Concrete example : N particles moving in one-dimensional space



$$U(\{q_\ell\}) = \sum_{i=1}^{N} V_{ext}(q_i) + \frac{1}{2}\sum_{i\neq j} v(q_i - q_j)$$

minimum : $\left.\dfrac{\partial U}{\partial q_i}\right|_{\vec{q}^{(0)}} = 0$

in general

$$q_i = q_i^{(0)} + x_i$$

$$M_i \ddot{q}_i = -\frac{\partial U}{\partial q_i}$$

$$M_i \ddot{x}_i = -\frac{\partial}{\partial x_i}\Big[U(\{q_i^{(0)}\}) + \frac{1}{4}\sum_{i\neq j} \left.\frac{\partial^2 v}{\partial q_i \partial q_j}\right|_0 x_i x_j$$

$$+ \frac{1}{2}\sum_i \frac{\partial^2 V_{ext}}{\partial q_i^2} x_i^2 + \dots \Big]$$

$$U_0 + \;= - \frac{\partial}{\partial x_i}\left[\frac{1}{2}\sum_{lm}\frac{\partial^2 U}{\partial x_l \partial x_m}\Big|_0 x_l x_m\right]$$

$$M_i \ddot{x}_i = -\sum_j \frac{\partial^2 U}{\partial x_i \partial x_j}\Big|_0 x_j + \mathcal{O}(x)^2$$

$$y_i = M_i x_i$$

$$\ddot{y}_i = -\sum_j \underbrace{\left(\frac{1}{M_i M_j}\frac{\partial^2 U}{\partial x_i x_j}\right)\Big|_0}_{A_{ij}} y_j + \mathcal{O}(x)^2$$

$$\boxed{\ddot{\vec{y}}(t) = -A\vec{y}}$$

$$\vec{y}(t) = \sum_{n=1}^{N} c_n \vec{u}_n e^{i\omega_n t} \qquad \vec{u}_m^{\,+}\cdot\vec{u}_n = \delta_{nm}$$

$\vec{u}_n$ orthonormal vectors

$$\vec{u}_m^{\,+}\cdot \sum_n c_n \vec{u}_n (-\omega_n^2) e^{-i\omega_n t} = -\vec{u}_m^{\,+}\sum_n c_n e^{-i\omega_n t} A\vec{u}_n$$

$$-\omega_m^2 c_m = -\sum_n c_n e^{-i(\omega_n-\omega_m)t}\, \underbrace{\vec{u}_m^{\,+} A \vec{u}_n}_{\delta_{nm}\lambda_m}$$

λ_m eigenvalue of A

$$A \vec{u}_n = \lambda_n \vec{u}_n$$

$$-\omega_m^2 C_m = -C_m \lambda_m$$

1) $\lambda_m = \omega_m^2 \geq 0$

$\underline{\underline{A}}$ is semi-positive definite

2) $\exists \lambda_p < 0$ $\qquad \omega_p^2 = -|\lambda_p|$

$$\omega_p = \pm i |\lambda_p|^{1/2}$$

$$e^{i\omega_p t} \to e^{|\lambda_p|^{1/2} t}$$

A) Full diagonalization of A

Python $\to$ LAPACK $\leftarrow$

Matlab

Mathematica

....

QR decomposition

property of A Hermitian

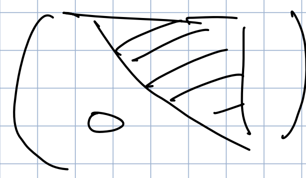
Scaling of full diagonalization of $N \times N$ matrix

$$T \sim O(N^3)$$

$$\underbrace{A = QR}_{T \sim O(N^3)}$$

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

R is upper triangular



$$A_1 = RQ = Q_1 R_1$$

$$= Q^\dagger Q A_1 = Q^\dagger Q R Q = Q^\dagger A Q$$

$$A_2 = R_1 Q_1 = Q_1^\dagger A_1 Q_1 = Q_1^\dagger Q^\dagger A Q Q$$

...

$$A_n \simeq \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$$

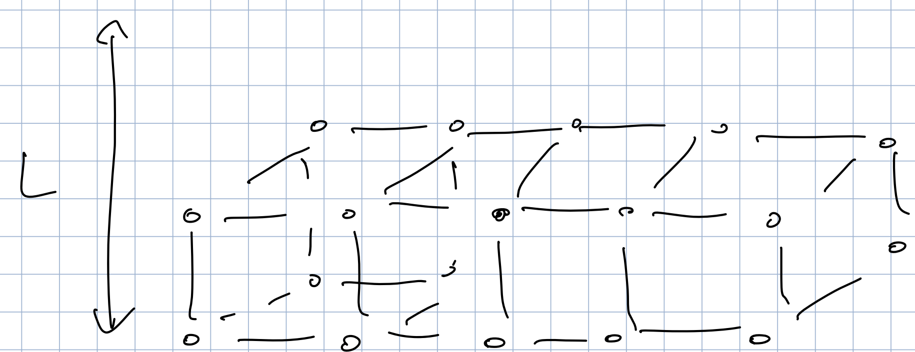
RAM is where you store your variables

n Gbytes (n = 8)

1 number = 8 bytes

$$N^2 \le \frac{\cancel{8} \cdot 10^9}{\cancel{8}} = 10^9$$

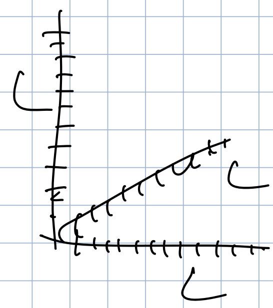
$$N \le 10^{9/2} \simeq 32000$$



$$N = 3L^3 \leq 32000$$

$$L \leq \sqrt[3]{\frac{32000}{3}} \approx 22$$

<u>quantum particle in 3d</u>



$$D = L^3$$

$$L \leq \sqrt[3]{32000}$$

$$\approx 32$$

<u>two quantum particles in 3d</u>

$$D = L^6$$

$$L \leq \sqrt[6]{32000} = 5.6$$

<u>"curse of dimensionality"</u>

<u>Tricks to alleviate the problem of storing the matrix A</u>

- 512 Gbytes (<u>using the hard disk</u>)

$8 \to 512 \qquad 70 \qquad \sqrt[3]{70} \approx 8$

- <u>matrix is sparse</u> = it has a lot of zero elements

Ex. $\underline{\mathcal{O}(N)}$ non-zero elements only

• <u>use symmetries</u>

A has a symmetry: $\exists\, V : V^\dagger V = \mathbb{1}$

$$\underbrace{V V^\dagger}_{\mathbb{1}} A V = V A$$

$$A V = V A \qquad [A, V] = 0$$

assuming that I know the eigenvectors / eigenvalues of V

$$V = \sum_{k=1}^{M} e^{i\phi_k} \sum_{l=1}^{d_k} \underbrace{|v_l^{(k)}\rangle \langle v_l^{(k)}|}_{\vec{v}_l^{(k)}\, \vec{v}_l^{(k)\dagger}}$$

$$V|v_l^{(k)}\rangle = e^{i\phi_k} |v_l^{(k)}\rangle$$

$$\langle v_l^{(k)} | \overbrace{A}^{k=k'} | v_{l'}^{(k')} \rangle \sim \delta_{kk'}$$

$$A = \begin{pmatrix} A_{k=1} & & & \\ & A_{k=2} & & \\ & & \ddots & \\ & & & A_{k=M} \end{pmatrix}$$

B) "Partial diagonalization"

Search for the extremal eigenvalue

$\lambda_1, \lambda_2, \dots, \lambda_N$ of A

$\lambda_{min} = \min_i \lambda_i = \lambda_1$

$\boxed{\text{Power method}}$

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

$\lambda_1 < \lambda_2 < \lambda_3 < \dots < \lambda_N$

$|\lambda_1 - \sigma| > |\lambda_2 - \sigma| \geq \dots \geq |\lambda_N - \sigma|$

$\lambda_1 \qquad \lambda_2 \qquad \lambda_N$

$\lambda_i - \sigma \to \lambda_i$

$|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_N|$

$\vec{u}$ trial approximation to $\vec{v}_1$

$\vec{u}^{\,t} \cdot \vec{v}_1 \neq 0$

$$\vec{u} = \sum_{k=1}^{N} c_k \vec{v}_k$$

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

$$A^M \vec{u} = c_1 \lambda_1^M \vec{v}_1 + \sum_{k\geq 2}^{N} c_k \lambda_k^M \vec{v}_k$$

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

$M \gg 1$

$\to 0$

$$A^M \vec{u} = c_1 \lambda_1^M \left[\vec{v}_1 + \cancel{\sum_{n\geq 2}^{N} c_n \left(\frac{\lambda_n}{\lambda_1}\right)^M \vec{v}_n} \right]$$

$$\left|\frac{\lambda_n}{\lambda_1}\right| < 1 \qquad \uparrow$$

$$\left(\frac{\lambda_n}{\lambda_1}\right)^M = \mathrm{sign}\left(\left(\frac{\lambda_n}{\lambda_1}\right)^M\right) e^{-M\left|\log\left|\frac{\lambda_n}{\lambda_1}\right|\right|}$$

$$e^{-aM} \qquad a>0$$

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

rate of convergence

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

c) Krylov space approach (Lanczos approach)

$$K_M = \mathrm{span}\{\vec{u}, A\vec{u}, A^2\vec{u}, A^3\vec{u}, \ldots, A^{M-1}\vec{u}\}$$

Krylov space

M is sufficiently small

all Krylov vectors are linearly independent

$$\dim(K_M) = M$$

Gram-Schmidt orthogonalise the Krylov vectors

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

$$\beta_1 \vec{u}_1 = A\vec{u}_0 - (\vec{u}_0^{\dagger} A\vec{u}_0)\vec{u}_0 \qquad \|\vec{u}_1\| = 1$$

$$\beta_2 \vec{u}_2 = A\vec{u}_1 - (\vec{u}_1^{\dagger} A\vec{u}_1)\vec{u}_1 - (u_0^{\dagger} A\vec{u}_1)\vec{u}_0$$

$$\beta_3 \vec{u}_3 = A\vec{u}_2 - (\vec{u}_2^{\dagger} A\vec{u}_2)\vec{u}_2 - (\vec{u}_1^{\dagger} A\vec{u}_2)\vec{u}_1 - \cancel{(\vec{u}_0^{\dagger} A\vec{u}_2)}\vec{u}_0$$

$$(\vec{u}_2^{\dagger} \cdot A\vec{u}_0)^{*}$$

$$\beta_4 \vec{u}_4 = A\vec{u}_3 - (\vec{u}_3^{\dagger} A\vec{u}_3)\vec{u}_3 - (\vec{u}_2^{\dagger} A\vec{u}_3)\vec{u}_2$$

...

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

..

$$\beta_{M-1} \vec{u}_{M-1}$$

M - dimensional

$$A^{(M)} = \{ \vec{u}_l^{\dagger} A \vec{u}_k \}$$

$$\left.\begin{matrix} \vec{u}_{k+1}^{\dagger} A\vec{u}_k \\ \vec{u}_k^{\dagger} A\vec{u}_k \\ \vec{u}_{k-1}^{\dagger} A\vec{u}_k \end{matrix}\right\} \neq 0$$

$$= \begin{pmatrix} \vec{u}_0^\dagger A \vec{u}_0 & \vec{u}_1^\dagger A \vec{u}_0 & 0 & 0 & \\ \vec{u}_0^\dagger A \vec{u}_1 & \vec{u}_1^\dagger A \vec{u}_1 & \vec{u}_2^\dagger A \vec{u}_1 & 0 & 0 \\ 0 & \vec{u}_1^\dagger A \vec{u}_2 & \vec{u}_2^\dagger A \vec{u}_2 & \vec{u}_3^\dagger A \vec{u}_2 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$

$A^{(M)}$ $\quad M \times M \quad \Rightarrow$ diagonalize

$\lambda_1^{(M)}$ lowest eigenvalue of $A^{(M)}$

$$\boxed{\lambda_1^{(M)} \geq \lambda_1} \qquad \lambda_1^{(M)} = \frac{(\vec{v}_1^{(M)})^\dagger A \vec{v}_1^{(M)}}{(\vec{v}_1^{(M)})^\dagger \vec{v}_1^{(M)}}$$

$$\lambda_1 = \min_{\vec{v}} \frac{\vec{v}^\dagger A \vec{v}}{\vec{v}^\dagger \vec{v}}$$

$$\vec{v} = \sum_n c_n \vec{v}_n \qquad \lambda_1 < \dots < \lambda_N$$

$$\frac{\vec{v}^\dagger A \vec{v}}{\vec{v}^\dagger \vec{v}} = \frac{\sum_n |c_n|^2 \lambda_n}{\sum_n |c_n|^2} \geq \frac{\sum_n |c_n|^2 \lambda_1}{\sum_n |c_n|^2} = \lambda_1$$