

# Matrix product states

d sites

$$\mathcal{F}_d = \{ |s_1, \dots, s_d \rangle \mid s_i \in \{1, 2\} \} \cong \mathbb{C}^{2^d}.$$

$$|\Psi\rangle = \sum_s \psi(s_1, \dots, s_d) |s_1 \dots s_d \rangle.$$

SVD .

$$\psi(s_1, \underbrace{s_2, \dots, s_d}_{\text{group}}) = \sum_{i=1}^{a_1} (A_1(s_1))_i \hat{\psi}_i^{(1)}(s_2, \dots, s_d),$$

group

$$= A_1(s_1) \hat{\psi}^{(1)}(s_2, \dots, s_d)$$

$$\cdot = A_1(s_1) \frac{a_1}{a_0=1} \hat{\psi}^{(1)}_{a_1} \quad | \quad a_1 \leq 2.$$

$$\hat{\psi}_i^{(1)}(s_2, \dots, s_d) = \sum_{j=1}^{a_2} (A_2(s_2))_{ij} \hat{\psi}_j^{(2)}(s_3, \dots, s_d)$$

$$\Rightarrow \hat{\psi}^{(1)}(s_2, \dots, s_d) = A_2(s_2) \hat{\psi}^{(2)}(s_3, \dots, s_d)$$

$$a_1 \quad \boxed{\quad} \quad = a_1 \boxed{\quad} \quad | \quad a_2 \leq 2^2.$$

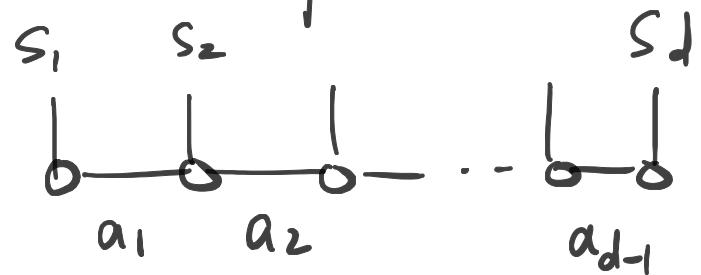
$$\Rightarrow \psi(s_1, \dots, s_d) = A_1(s_1) A_2(s_2) \cdots A_d(s_d).$$

$$A_i(s_i) \in \mathbb{C}^{a_{i-1} \times a_i}, \quad a_0 = a_d = 1.$$

$$a_i \leq 2^i$$

MPS.  $m = \max \{a_0, \dots, a_d\}$  bond dimension.

graphical representation



edge : matrix-matrix  
multiplication.

Useful scenario.

$f(s_1, \dots, s_d)$  well approximated by MPS

w. m. weakly depending on d.

$$\mathcal{F}_{m,d}^{\text{MPS}} = \left\{ A_1(s_1) \cdots A_d(s_d) \mid A_i \in \mathbb{C}^{a_{i-1} \times a_i}, a_0 = a_d = 1, a_i \leq m \right\}.$$

$$E_0 \leq \inf \langle \psi | H | \psi \rangle$$

$$\psi \in \mathcal{F}_{n,d}^{\text{MPS}}$$

$$\langle \psi | \psi \rangle = 1$$

$H$ : lattice Ham. Honian.

e.g. 1) Heisenberg.

$$H = \sum_{i=1}^{d-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \sum_{i=1}^d S_i^z S_{i+1}^z$$

DMRG: an algorithm to solve optimization problem. (2-site version)

Ex. 2-site

$$\psi(s_1, s_2) = A_1(s_1) B_2(s_2)$$

$$1 = a_0 \overline{\frac{a_1}{a_2}} \quad a_1 \Big| \quad a_1 = 2 \\ a_2 = 1,$$

$$\begin{matrix} 0 & | & 0 \\ L & & R \end{matrix}$$

$$|\phi_{\alpha}^{L(1)}\rangle = \sum_{s_1} A_1(s_1) |s_1\rangle ,$$

$$|\phi_{\beta}^{R(2)}\rangle = \sum_{s_2} B_2(s_2) |s_2\rangle ,$$

$$\delta_{\alpha, s_1} = A_1(s_1)$$

$$\delta_{\beta, s_2} = B_2(s_2)$$

$$|\Psi\rangle = \sum_{\alpha\beta} C_{\alpha\beta} |\phi_{\alpha}^{L(1)} \phi_{\beta}^{R(2)}\rangle$$

$$\langle \phi_{\alpha}^{L(1)} \phi_{\beta}^{R(2)} | \phi_{\alpha'}^{L(1)} \phi_{\beta'}^{R(2)} \rangle = \delta_{\alpha\alpha'} \delta_{\beta\beta'}$$

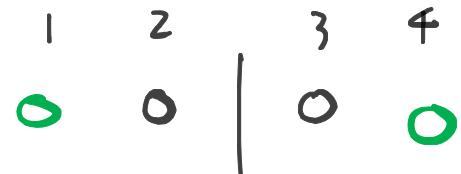
Solve  $\sum_{\alpha'\beta'} \langle \phi_{\alpha}^{L(1)} \phi_{\beta}^{R(2)} | H | \phi_{\alpha'}^{L(1)} \phi_{\beta'}^{R(2)} \rangle C_{\alpha'\beta'} = E C_{\alpha\beta}$

$$C_{\alpha\beta} \xrightarrow{SVD} A_1, B_2. \text{ trivial.}$$

$$\sum_{s_1} A_1(s_1)^* A_1(s_1) = \delta_{\alpha\alpha'}$$

$$\sum_{s_2} B_2(s_2) B_2^*(s_2) = \delta_{\beta\beta'}$$

Ex. 4-site.



$$|\tilde{\phi}_{\tilde{\alpha}}^{L(2)}\rangle = |\phi_{\alpha}^{L(1)}\rangle \otimes |S_2\rangle. \quad \tilde{\alpha} = (\alpha, s_2)$$

$$|\tilde{\phi}_{\tilde{\beta}}^{R(3)}\rangle = |S_3\rangle \otimes |\phi_{\beta}^{R(4)}\rangle. \quad \tilde{\beta} = (s_3, \beta)$$

$$\langle \tilde{\phi}_{\tilde{\alpha}}^{L(2)} \tilde{\phi}_{\tilde{\beta}}^{R(3)} | \tilde{\phi}_{\tilde{\alpha}'}^{L(2)} \tilde{\phi}_{\tilde{\beta}'}^{R(3)} \rangle = \delta_{\tilde{\alpha}\tilde{\alpha}'} \delta_{\tilde{\beta}\tilde{\beta}'}$$

extended basis

$$|\Psi\rangle = \sum_{\tilde{\alpha}\tilde{\beta}} \tilde{C}_{\tilde{\alpha}\tilde{\beta}} |\phi_{\tilde{\alpha}}^{L(z)} \phi_{\tilde{\beta}}^{R(z)}\rangle$$

$$\sum_{\tilde{\alpha}'\tilde{\beta}'} \langle \phi_{\tilde{\alpha}}^{L(z)} \phi_{\tilde{\beta}}^{R(z)} | H | \phi_{\tilde{\alpha}'}^{L(z)} \phi_{\tilde{\beta}'}^{R(z)} \rangle \tilde{C}_{\tilde{\alpha}'\tilde{\beta}'}^* = \in \tilde{C}_{\tilde{\alpha}'\tilde{\beta}'}^*$$

superblock Hamiltonian

SVD

$$\tilde{C}_{\tilde{\alpha}\tilde{\beta}} = \sum_{k=1}^m U_{\tilde{\alpha}k} \sigma_k V_{\tilde{\beta}k}^*. \quad (m \leq 2^z)$$

Link w. MPS?

$$(A_z(s_z))_{\alpha', k} = U_{(\alpha', s_z), k}. \quad k : \text{bond dimension}$$

$$(B_z(s_z))_{k, \beta'} = V_{(s_z, \beta'), k}^*. \quad k=1, -; m$$

$$|\phi_{\alpha}^{L(2)}\rangle = \sum_{\alpha'=1}^{\alpha_1} \sum_{s_2} (A_2(s_2))_{\alpha', \alpha} |\phi_{\alpha'}^{L(1)}\rangle \otimes |s_2\rangle.$$

$$\alpha = 1, \dots, \alpha_2 = m$$

$$|\phi_{\beta}^{R(3)}\rangle = \sum_{\beta'=1}^{\alpha_3} \sum_{s_3} (B_3(s_3))_{\beta, \beta'} |s_3\rangle \otimes |\phi_{\beta'}^{R(4)}\rangle$$

$$\beta = 1, \dots, b_3 = m.$$

$$\langle \phi_{\alpha}^{L(2)} | \phi_{\alpha'}^{L(2)} \rangle = \sum_{S_2} \left( A_2^*(S_2) A_2(S_2) \right)_{\alpha, \alpha'} = \delta_{\alpha \alpha'},$$

$$\langle \phi_{\beta}^{R(3)} | \phi_{\beta'}^{R(3)} \rangle = \sum_{S_3} \left( B_3(S_3) B_3^*(S_3) \right)_{\beta, \beta'} = \delta_{\beta \beta'}.$$

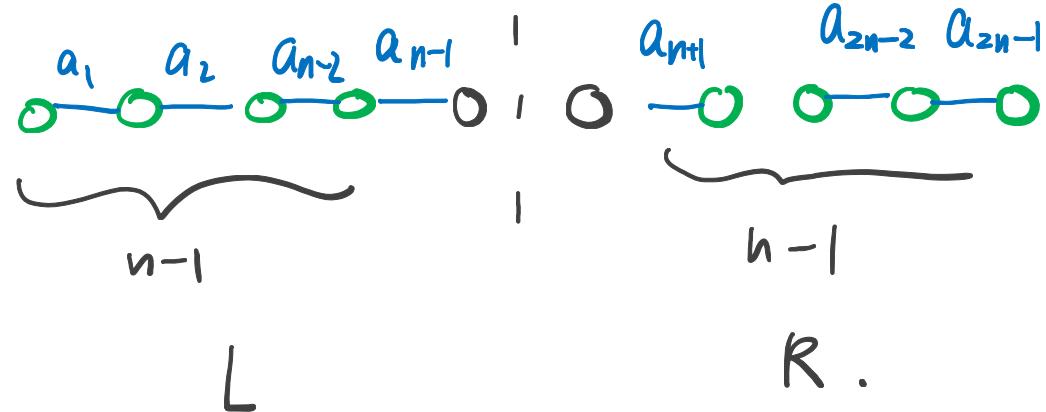
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orthogonality of U, V.

$$\begin{aligned}
 (\text{exer}) \quad |\psi\rangle &= \sum_{\alpha \beta} c_{\alpha \beta} |\phi_{\alpha}^{L(2)} \phi_{\beta}^{R(3)}\rangle \\
 &= \sum_{S_1 \dots S_4} A_1(S_1) A_2(S_2) C B_3(S_3) B_4(S_4)
 \end{aligned}$$

$$C_{\alpha \beta} = \sigma_k \delta_{\alpha k} \delta_{\beta k}.$$

$2n$  sites



$$|\phi_{\alpha}^{L(n-1)}\rangle \quad | \phi_{\beta}^{R(n+2)}\rangle \quad \text{given . orthogonal.}$$

$$\alpha = 1, \dots, a_{n-1} \quad \beta = 1, \dots, a_{n+1}$$

$$|\tilde{\phi}_{\alpha}^{L(n)}\rangle = |\phi_{\alpha}^{L(n-1)}\rangle \otimes |s_n\rangle, \quad \tilde{\alpha} = (\alpha, s_n)$$

$$|\tilde{\phi}_{\beta}^{R(n+1)}\rangle = |s_{n+1}\rangle \otimes |\phi_{\beta}^{R(n+2)}\rangle, \quad \tilde{\beta} = (s_{n+1}, \beta).$$

$$\sum_{\alpha' \beta'} \left\langle \overset{\sim}{\phi}_{\tilde{\alpha}}^{L(n)} \overset{\sim}{\phi}_{\tilde{\beta}}^{R(n+1)} \mid H \right. \mid \left. \overset{\sim}{\phi}_{\tilde{\alpha}'}^{L(n)} \overset{\sim}{\phi}_{\tilde{\beta}'}^{R(n+1)} \right\rangle \tilde{C}_{\tilde{\alpha}' \tilde{\beta}'}$$

$$= \tilde{C}_{\tilde{\alpha}' \tilde{\beta}'} E$$

$$\tilde{C}_{\tilde{\alpha} \tilde{\beta}} \approx \sum_k U_{\tilde{\alpha} k} \sigma_k V_{\tilde{\beta} k}^*, \quad k=1, \dots, m$$

$$(A_n(s_n))_{\alpha', k} = \bigcup_{(\alpha', s_n), k}$$

$$(B_{n+1}(s_{n+1}))_{k, \beta'} = V_{(s_{n+1}, \beta'), k}^*$$

$$\sum_n (A_n(s_n))^* (A_n(s_n)) = U^* U = I_m$$

$$\sum_{S_{n+1}} \left( B_{n+1}(S_{n+1}) \right) \left( B_{n+1}(S_{n+1}) \right)^* = V^* V = I_m.$$

$$|\phi_{\alpha}^{L(n)}\rangle = \sum_{\alpha'} \sum_{S_n} \left( A_n(S_n) \right)_{\alpha', \alpha} |\phi_{\alpha'}^{L(n)}\rangle \otimes |S_n\rangle$$

$$|\phi_{\beta}^{R(n+1)}\rangle = \sum_{\beta'} \sum_{S_{n+1}} \left( B_n(S_{n+1}) \right)_{\beta, \beta'}, |S_{n+1}\rangle \otimes |\phi_{\beta'}^{R(n+1)}\rangle$$

$$\langle \phi_{\alpha}^{L(n)} | \phi_{\alpha'}^{L(n)} \rangle = \delta_{\alpha \alpha'}$$

$$\langle \phi_{\beta}^{R(n+1)} | \phi_{\beta'}^{R(n+1)} \rangle = \delta_{\beta \beta'}$$

# Infinite system DMk G

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Efficient computation of

$$\langle \phi_{\tilde{\alpha}}^{L(n)} \phi_{\tilde{\beta}}^{k(n+1)} | H | \tilde{\phi}_{\tilde{\alpha}}^{L(n)} \tilde{\phi}_{\tilde{\beta}}^{R(n+1)} \rangle.$$

$$H = \sum_{i=1}^{2n-1} \vec{S}_i \cdot \vec{S}_{i+1}$$
$$=: \sum_{i=1}^{2n-1} O_{L,i} O_{R,i}$$

Case 1.

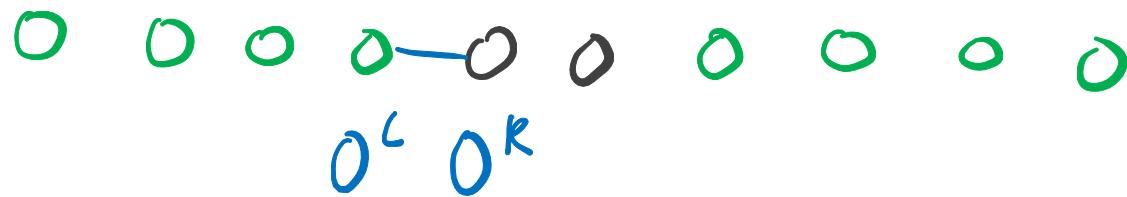


$$(\star) \quad \left\langle \phi_{\tilde{\alpha}}, \phi_{\tilde{\beta}}^{\text{R}(n+1)} \right| O^L O^R | \phi_{\tilde{\alpha}}^{\text{L}(n)} \phi_{\tilde{\beta}}^{\text{R}(n+1)} \right\rangle$$

$$= \delta_{\tilde{\beta} \tilde{\alpha}} \delta_{s'_n s_n} \left\langle \phi_{\tilde{\alpha}'}^{\text{L}(n)} | O^L O^R | \phi_{\tilde{\alpha}}^{\text{L}(n-1)} \right\rangle.$$

↑  
reuse       $\langle O^L O^R \rangle_{\tilde{\alpha}' \tilde{\alpha}}^{\text{L}(n-1)}$

Case 2 .



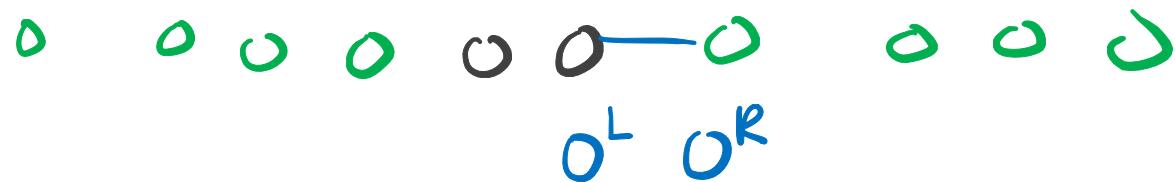
$$\begin{aligned}
 & \langle \tilde{\phi}_{\tilde{\alpha}'}^{L(n)} | \tilde{\phi}_{\tilde{\beta}'}^{R(n+1)} | O^L O^R | \tilde{\phi}_\alpha^{L(n)} | \tilde{\phi}_{\tilde{\beta}}^{R(n+1)} \rangle \\
 = & \langle \phi_{\alpha'}^{L(n-1)} | O^L | \phi_\alpha^{L(n-1)} \rangle \langle s'_n | O^R | s_n \rangle \delta_{\tilde{\beta}' \tilde{\beta}} \\
 & \quad \uparrow \quad \uparrow \\
 & \quad \text{reuse} \quad \text{direct compute} \\
 & \quad \langle O^L \rangle_{\alpha' \alpha}^{L(n-1)}
 \end{aligned}$$

Case 3.

$$\begin{array}{ccccccccc}
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & & & & O^L & O^R & & &
 \end{array}$$

$$(\star) = \langle s'_n | O^L | s_n \rangle \langle s'_{n+1} | O^R | s_{n+1} \rangle \delta_{\alpha' \alpha} \delta_{\beta' \beta}$$

Case 4.



Same case 2



Same case 1.

Update basis .  $\langle 0^L \rangle \rightarrow \langle s'_n | 0^L | s_n \rangle$

$$\langle 0^L 0^k \rangle_{\alpha' \alpha}^{L(n-1)} \delta_{s'_n s_n} \rightarrow \langle 0^L 0^k \rangle^{L(n)}$$

$$1. \langle 0^L 0^R \rangle^{L(n)} = U^* \left( \langle 0^L 0^R \rangle^{L(n-1)} \otimes I_2 \right) U$$

$$2. \langle 0^L \rangle^{L(n)} = U^* \left( I_{a_{n-1}} \otimes \langle 0^L \rangle \cdot \right) U.$$

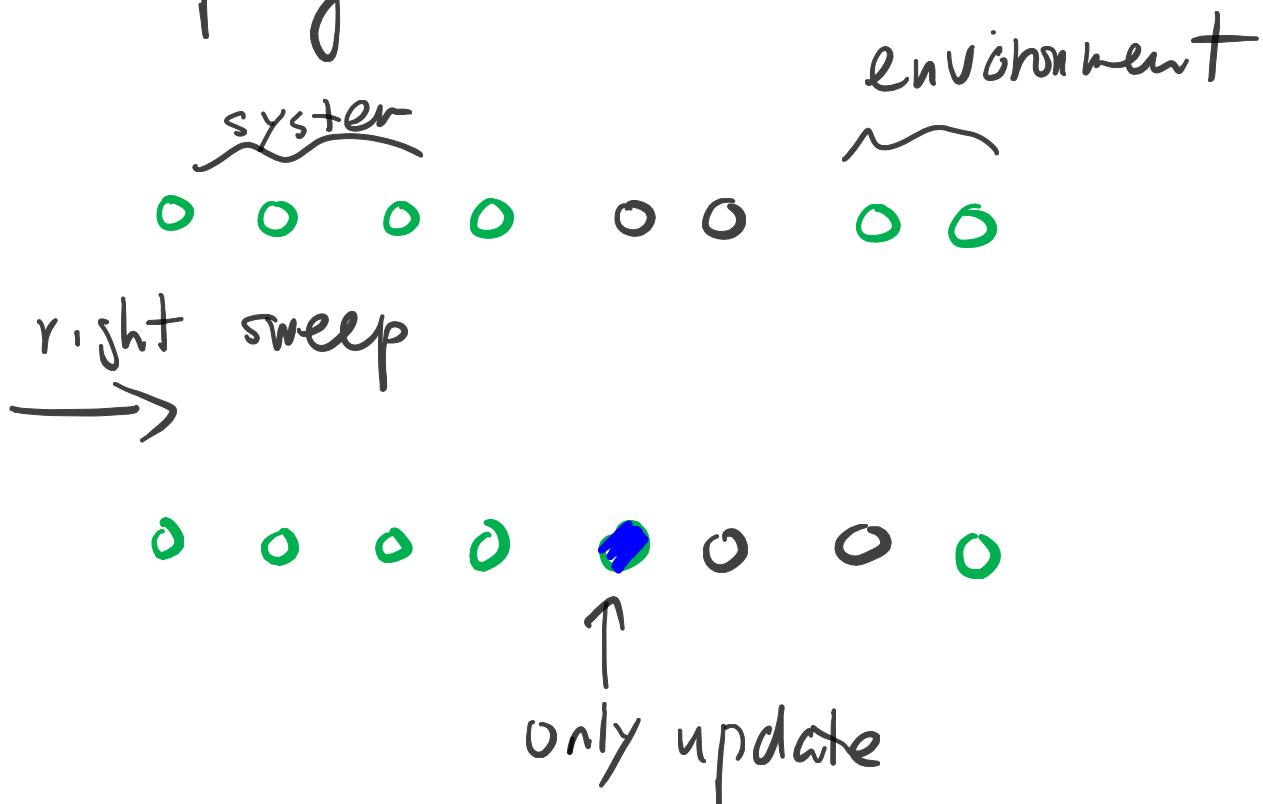
$$4. \langle 0^R \rangle^{R(n+1)} = V^* \left( \langle 0^R \rangle \otimes I_{a_{n+2}} \right) V$$

$$5. \langle 0^L 0^R \rangle^{R(n+1)} = V^* \left( I_2 \otimes \langle 0^L 0^R \rangle^{R(n+2)} \right) V$$

3. intact .

Finite system DMRG.

sweeping



then left sweep.

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fermionic system.

$$H = -t \sum_{i=1}^N \sum_{\sigma} (c_{i\sigma}^+ c_{i+\sigma} + h.c.) + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow}.$$

# Jordan-Wigner transformation.

$| \uparrow \downarrow | \downarrow \uparrow | 2\uparrow 2\downarrow \dots | N\uparrow N\downarrow$  fermions

1 2 3  $zN$ . spins.

$$C_{it}^+ = \sum^{(i-1) \leftarrow} \otimes \left( A^+ \otimes I \right) \otimes I^{(i+1), \rightarrow}$$

$$Z^{j,<} = \underbrace{Z \otimes Z \otimes \cdots \otimes Z}_{2j}$$

$$I^{j,\rightarrow} = \underbrace{I \otimes \cdots \otimes I}_{2(N-j+1)}$$

$$C_{i\downarrow}^+ = Z^{(i-1),<} \otimes (I \otimes A^+) \otimes I^{i+1,\rightarrow}.$$

$C_{i\uparrow}, C_{i\downarrow}$  similar.

$$\begin{aligned}
C_{i\uparrow}^+ C_{i+1\uparrow} &= \left( Z^{i-1,\leftarrow} \otimes (A^+ \otimes I) \otimes (I \otimes I) \otimes I^{i+2,\rightarrow} \right) \\
&\quad \left( Z^{i-1,\leftarrow} \otimes (Z \otimes Z) \otimes (A \otimes I) \otimes I^{-i+2,\rightarrow} \right) \\
&= I^{i-1,\leftarrow} \otimes (A^+ Z \otimes Z) \otimes (A \otimes I) \otimes I^{i+2,\rightarrow} \\
&\qquad O^L \qquad O^R.
\end{aligned}$$

$$\begin{aligned}
C_{i+1,\uparrow}^+ C_{i,\uparrow} &= I^{i-1,\leftarrow} \otimes (Z A \otimes Z) \otimes (A^+ \otimes I) \otimes I^{i+2,\rightarrow} \\
&\qquad O^L \qquad O^R
\end{aligned}$$

Similar for other terms.

Use previous alg. Note distinction

between left and right side

( $\geq \otimes \geq$  always on the left)

Notebook.

