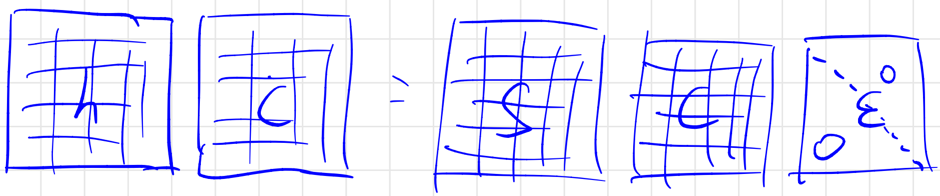
Discussion 3

$$(|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, \cdots |\psi_n\rangle) = (|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle \cdots |\phi_n\rangle)\begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1n} \\ C_{21} & C_{22} & \cdots & C_{2n} \\ C_{31} & C_{32} & \cdots & C_{3n} \\ \vdots & \vdots & & \vdots \\ C_{n1} & C_{n2} & \cdots & C_{nn} \end{pmatrix}$$

minimize $\langle \Psi(x_1, x_2, \cdots x_n) | \hat{H} | \Psi(x_1, x_2, \cdots x_n) \rangle$

$$\Longleftrightarrow \sum_i \langle \psi_i | \hat{h}_{eff} | \psi_i \rangle \qquad hC = C\varepsilon$$

$$\Longleftrightarrow \quad hC = SC\varepsilon$$



$$h_{\mu\nu} = \langle \phi_\mu | \hat{h}_{eff} | \phi_\nu \rangle \qquad \underline{C_{\mu i}}$$

$$S_{\mu\nu} = \langle \phi_\mu | \phi_\nu \rangle$$

In Hukel theory,

$$h_{\mu\nu} = \frac{K}{2}[h_{\mu\mu} + h_{\nu\nu}]$$

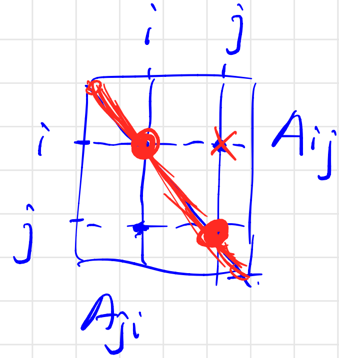
$$\hat{h}_{eff} = -\frac{1}{2}\nabla_i^2 + V_{eff}(\vec{r})$$

$$\langle \phi_\mu | \hat{h}_{eff} | \phi_\nu \rangle = \int d\vec{r}\, \phi_\mu(\vec{r}) \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}\phi_\nu(\vec{r}) - \frac{1}{2}\frac{\partial^2}{\partial y^2}\phi_\nu(\vec{r}) - \frac{1}{2}\frac{\partial^2}{\partial z^2}\phi_\nu(\vec{r}) + V_{eff}(\vec{r})\phi_\nu(\vec{r}) \right]$$

$$h_{\mu\nu} = \frac{K}{2}\left(h_{\mu\mu} + h_{\nu\nu}\right)$$

known

$$A_{ij} = A_{ji}$$



$$h_{\nu\mu} = \frac{K}{2}\left(h_{\nu\nu} + h_{\mu\mu}\right) = \frac{K}{2}\left(h_{\mu\mu} + h_{\nu\nu}\right) = h_{\mu\nu}$$

$$S_{\mu\nu} = \int d\vec{r}\, \phi_\mu(\vec{r})\phi_\nu(\vec{r}) = \int d\vec{r}\, \phi_\nu(\vec{r})\phi_\mu(\vec{r}) = S_{\nu\mu}$$

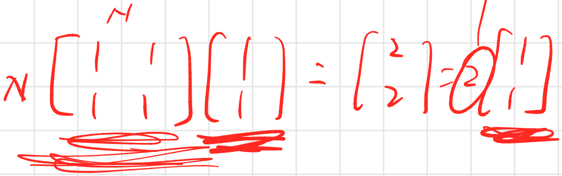
$$hC = SC\varepsilon \iff \underbrace{S^{-1}h}_{A}\, C = C\varepsilon$$

$$h^T = h, \quad S^T = S$$

$$AC = C\varepsilon$$

$$A^T = (S^{-1}h)^T = h^T (S^{-1})^T \neq A$$

$$\boxed{C}$$



$$hC = SC\varepsilon \quad ?$$

$$S^{-\frac{1}{2}} h C = S^{-\frac{1}{2}} S C \varepsilon$$

$$S^{-\frac{1}{2}} h S^{-\frac{1}{2}} S^{\frac{1}{2}} C = S^{\frac{1}{2}} C \varepsilon$$

eigenvector matrix

$$A^T = A \qquad A = U \Lambda U^T$$

$$\Lambda = \begin{bmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \lambda_3 \end{bmatrix} \qquad U^T U = I$$

$$f(A) = U f(\Lambda) U^T$$

$$f(\Lambda) = \begin{bmatrix} f(\lambda_1) & & 0 \\ & f(\lambda_2) & \\ 0 & & f(\lambda_3) \ddots \end{bmatrix}$$

$$S^{-\frac{1}{2}} = U \begin{bmatrix} s_1^{-\frac{1}{2}} & & \\ & s_2^{-\frac{1}{2}} & \\ & \ddots & s_n^{-\frac{1}{2}} \end{bmatrix} U^T$$

where $S = U s U^T$

eigenvalues of S

$$hC = SC\varepsilon$$

$$S^{-\frac{1}{2}} h C = S^{-\frac{1}{2}} S C \varepsilon \qquad S^{-\frac{1}{2}} S = S^{\frac{1}{2}}$$

$$\underbrace{S^{-\frac{1}{2}} h S^{-\frac{1}{2}}}_{h'} \underbrace{S^{\frac{1}{2}} C}_{C'} = \underbrace{S^{\frac{1}{2}} C}_{C'} \varepsilon$$

$$\Rightarrow \boxed{h' C' = C' \varepsilon}$$

$$h' = S^{-\frac{1}{2}} h S^{-\frac{1}{2}} \qquad C' = S^{\frac{1}{2}} C$$

$$h'^{T} = \left(S^{-\frac{1}{2}} h S^{-\frac{1}{2}}\right)^{T}$$
$$= \left(S^{-\frac{1}{2}}\right)^{T} h^{T} \left(S^{-\frac{1}{2}}\right)^{T}$$
$$= S^{-\frac{1}{2}} h S^{-\frac{1}{2}} = h'$$

solve solve

$$h' C' = C' \varepsilon$$

$$C = S^{-\frac{1}{2}} C'$$

① Construct S, h

② arma::vec S_eval; arma::mat S_evec;
arma::eig_sym(S_eval, S_evec, S)

arma::mat $S^{-\frac{1}{2}}$ = S_evec * S_eval$^{-\frac{1}{2}}$ * transpose(S_evec)

$$S^{\frac{1}{2}} = S\_evec * S\_eval^{\frac{1}{2}} * transpose(S\_evec)$$

③ arma h_prime = $S^{-\frac{1}{2}} * h * S^{-\frac{1}{2}}$

eig_sym(ε , C_prime, h_prime)

④ arma C = $S^{-\frac{1}{2}}$ * C_prime ;

$$S^{-\frac{1}{2}} S^{\frac{1}{2}} = I$$

$$S^{-\frac{1}{2}} S^{\frac{1}{2}} = U \begin{pmatrix} s_1^{-\frac{1}{2}} & & 0 \\ & s_2^{-\frac{1}{2}} & \\ 0 & & \ddots \; s_n^{-\frac{1}{2}} \end{pmatrix} \underbrace{U^T U}_{I} \begin{pmatrix} s_1^{\frac{1}{2}} & & 0 \\ & s_2^{\frac{1}{2}} & \\ 0 & & \ddots \; s_n^{\frac{1}{2}} \end{pmatrix} U^T$$

$$= U \begin{pmatrix} s_1^{-\frac{1}{2}} & & 0 \\ & s_2^{-\frac{1}{2}} & \\ 0 & & \ddots \; s_n^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} s_1^{\frac{1}{2}} & & 0 \\ & s_2^{\frac{1}{2}} & \\ 0 & & \ddots \; s_n^{\frac{1}{2}} \end{pmatrix} U^T$$

$$= U \begin{pmatrix} s_1^{-\frac{1}{2}} s_1^{\frac{1}{2}} & & 0 \\ & s_2^{-\frac{1}{2}} s_2^{\frac{1}{2}} & \\ 0 & & \ddots \; s_n^{-\frac{1}{2}} s_n^{\frac{1}{2}} \end{pmatrix} U^T$$

$$= U \underbrace{\begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & \ddots \; 1 \end{pmatrix}}_{I} U^T = UU^T = UU^{-1} = I$$

$$U^T U = I \iff U^T = U^{-1}$$