

| dict\_df = {w1s1: "df"}

Matrix distance

- for archive\_XYZ


- o ~~filtro para a homom~~

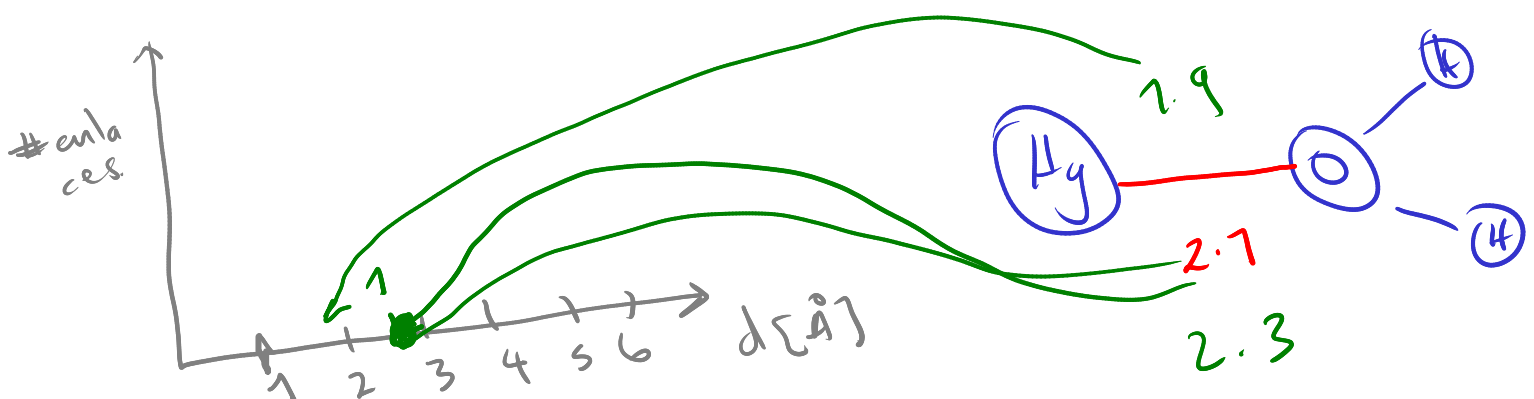
	Hg	O	H	
Hg	0	2.0	3.2	3.7
O	x	0	x	x
H	x	y	0	y
	a	b	c	d

$$i_j \rightarrow j_i$$

def distance\_matrix (dict\_df, ...)

\* return dict\_dMatrix {wts1:  $\mathbb{F}$ }


 symbols    ↓   ↓



```
def rda (dict_coord, dict_dMat)
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return dict\_rda = {wts1:  $\begin{bmatrix} w_1 & w_2 \\ d_1 & d_2 \end{bmatrix}$ }

$$\begin{aligned} dr &= 0.07 \text{ A} \\ r_0 &= 0.5 \text{ A} \\ r_f &= 3.0 \text{ A} \end{aligned}$$

inbin

$$0.5 \rightarrow 0.51, \dots$$
$$\begin{aligned} d\theta &= \delta\theta \\ \theta_0 &= \\ \theta_f &= \end{aligned}$$

① Construir el grid para todos  $\Rightarrow$  distancias  
 $\Rightarrow$  ángulo plano  
 $\Rightarrow$  ángulo diedral

② Construir función para matriz de distancia.  $H_y \quad O \quad H$   
 $dict = \{w1s1: "d_F"\} \Rightarrow d_F = \begin{matrix} & H_y & O & H \\ H_y & d_{H_y H_y} & d_{H_y O} & d_{H_y H} \\ O & & d_{O O} & d_{O H} \\ H & & & d_{H H} \end{matrix}$

③ Construir función 2DA

$dict = \{w1s1: "d_F"\} \Rightarrow d_F =$

