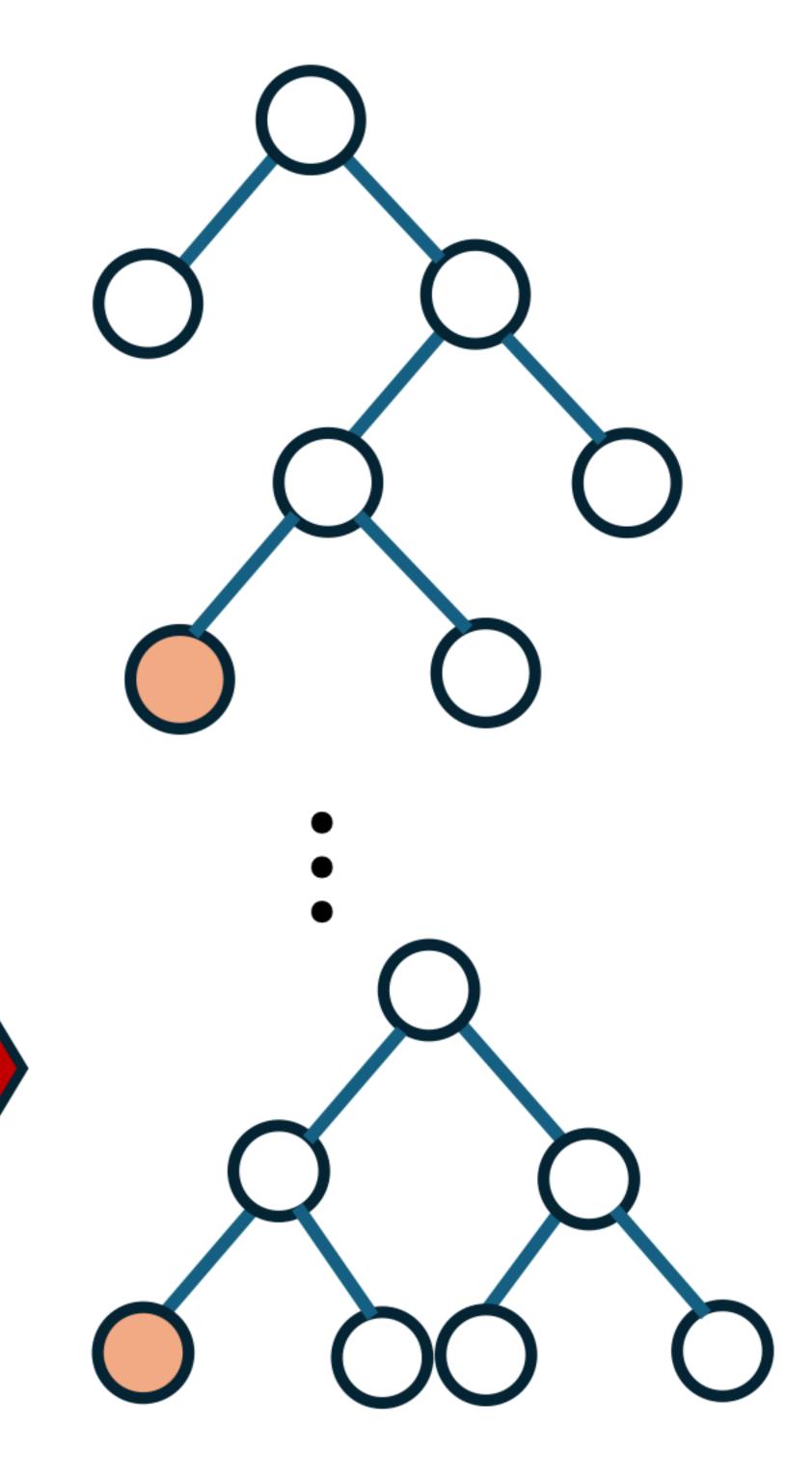


N=2 Persistent homology  $d^2 = 0$   $\beta_0, \beta_1, \beta_2$ 

 $a^{3} = 0$  N=3  $\beta_{0,1}, \beta_{1,1}, \beta_{2,1}$   $\beta_{0,2}, \beta_{1,2}, \beta_{2,2}$ 

 $d^{5} = 0$   $\beta_{0,1}, \beta_{1,1}, \beta_{2,1}$   $N=5 \quad \beta_{0,2}, \beta_{1,2}, \beta_{2,2}$   $\beta_{0,3}, \beta_{1,3}, \beta_{2,3}$   $\beta_{0,4}, \beta_{1,4}, \beta_{2,4}$ 

Persistent Mayer homology



Training or predictions

Protein-ligand complex

Elementspecific
atom groups

Elementinteractive filtration Persistent
Mayer homology
features

Machine Learning predictions