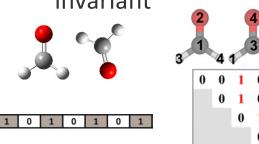


Input features

- w/ or w/o 3D coord.
- Descriptors such as graphs, fingerprints, ...
- Rotation/permutation 'invariant'



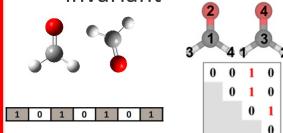
Regression
Multivariate model
(Week 11)
Machine learning
(Week 13)
Deep learning
(Week 14),
etc.

Various physical/chemical properties (experimental, calculated)

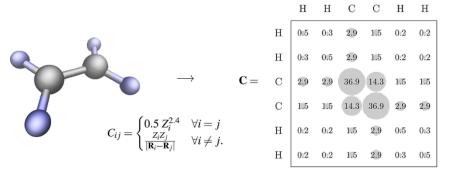
Handling big data (Week 12)

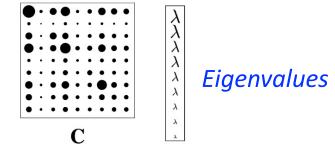
Input features

- w/ or w/o 3D coord.
- Descriptors such as graphs, fingerprints, ...
- Rotation/permutation 'invariant'



Input features using 3D coordinates

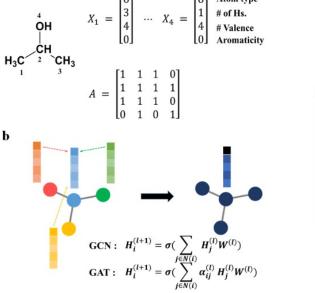


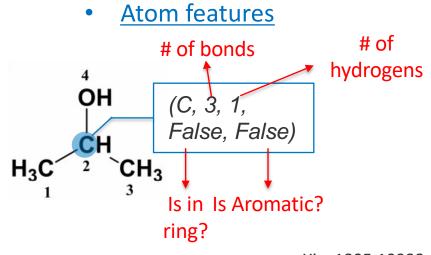


$$C_{ij} = \begin{cases} 0.5 Z_i^{2.4} & \forall i = j \\ \frac{Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} & \forall i \neq j. \end{cases}$$

J. Chem. Theory Comput., 2013, 9, 3404.

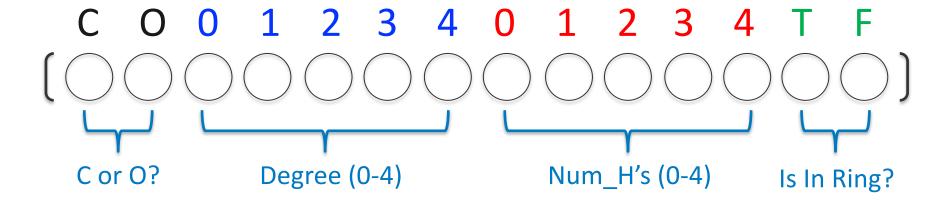
Input features w/o 3D coordinates





arXiv: 1805.10988v2

One-hot Vector - Example



e.g.) Carbon, Degree 4, 3 hydrogens, not in the ring (1,0, 0,0,0,0,1, 0,0,0,1,0, 0, 1)