

Cormorant: COvaRiant MOleculaR Artificial Neural neTworks

Spotlight Presentation

Brandon M. Anderson ^{*,†} Truong Son Hy ^{*} Risi Kondor ^{*,†,‡}

^{*}Department of Computer Science
The University of Chicago

[†]Department of Statistics
The University of Chicago

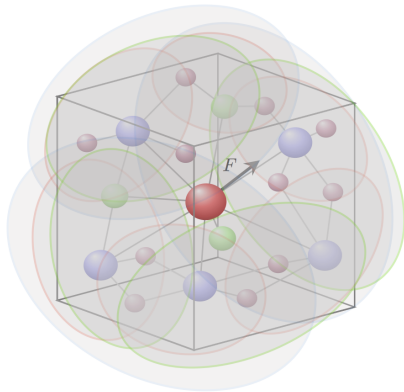
[‡]Center for Computational Mathematics
Flatiron Institute

[‡]Atomwise

2019 Conference on Neural Information Processing Systems

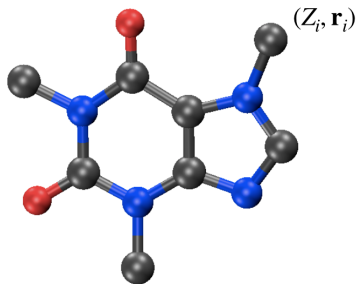


Learning on molecular data



$$F(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_m)$$

Learn on molecules:

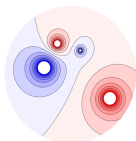


Data has built-in symmetry
→ Use covariant activations!

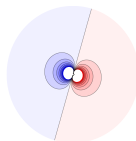


The multipole expansion

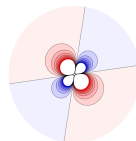
$$\sum_i Z_i/|\mathbf{r} - \mathbf{r}_i| = Q_0 Y^0(\hat{\mathbf{r}})/r + Q_1 Y^1(\hat{\mathbf{r}})/r^2 + Q_2 Y^2(\hat{\mathbf{r}})/r^3 + \dots$$



monopole



dipole



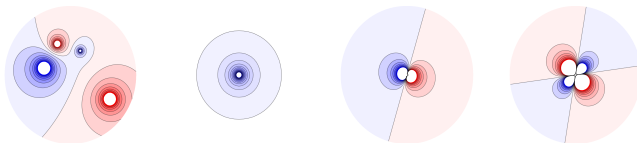
quadrupole

- Q_ℓ : ℓ -th multipole moment
- Y^ℓ : ℓ -th spherical harmonic



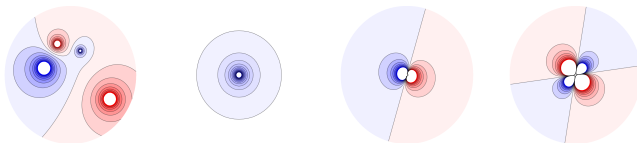
Covariant rotations

Consider a 90° CCW-rotation R :

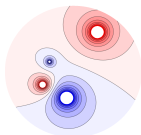


Covariant rotations

Consider a 90° CCW-rotation R :

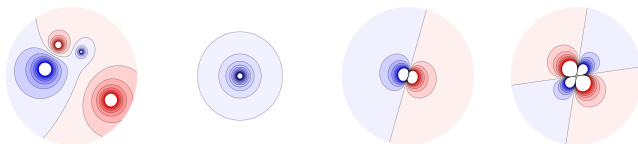


After a rotation:

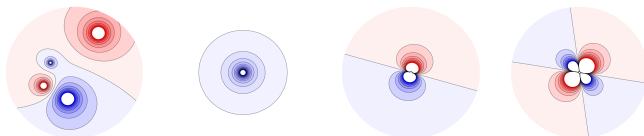


Covariant rotations

Consider a 90° CCW-rotation R :



After a rotation:

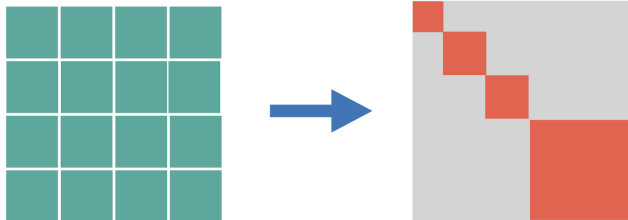


All moments rotate “covariantly”:

$$Q_\ell \rightarrow D^\ell(R)Q_\ell$$



Clebsch-Gordan Transformation



Group theory:

$$D^{\ell_1}(R) \otimes D^{\ell_2}(R) = C_{\ell_1, \ell_2}^\dagger \left[\bigoplus_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2} D^\ell(R) \right] C_{\ell_1, \ell_2}$$

$D^\ell(R)$: Wigner-D (Rotation) matrix

$C_{\ell_1 \ell_2}$: Clebsch-Gordan matrix

$R \in \text{SO}(3)$



SO(3)-Vectors

SO(3)-Vector: $F_{\ell,c}$

- Transforms covariantly: $F_{\ell,c} \rightarrow D^\ell(R)F_{\ell,c}$



SO(3)-Vectors

SO(3)-Vector: $F_{\ell,c}$

- Transforms covariantly: $F_{\ell,c} \rightarrow D^\ell(R)F_{\ell,c}$

Limited operations available:

- Linearly mixed: $\sum_c F_{\ell,c'} W_{c'c}$



SO(3)-Vector: $F_{\ell,c}$

- Transforms covariantly: $F_{\ell,c} \rightarrow D^\ell(R)F_{\ell,c}$

Limited operations available:

- Linearly mixed: $\sum_c F_{\ell,c'} W_{c'c}$
- Clebsch-Gordan product: $F_{\ell_1,c} \otimes_{\text{CG}} F_{\ell_2,c} = C_{\ell_1\ell_2} \left[\bigoplus_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2} F_{\ell,c} \right]$



SO(3)-Vector: $F_{\ell,c}$

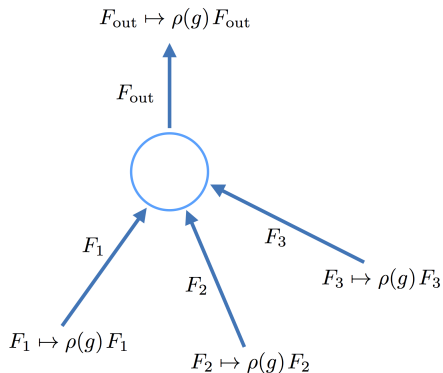
- Transforms covariantly: $F_{\ell,c} \rightarrow D^\ell(R)F_{\ell,c}$

Limited operations available:

- Linearly mixed: $\sum_c F_{\ell,c'} W_{c'c}$
- Clebsch-Gordan product: $F_{\ell_1,c} \otimes_{\text{CG}} F_{\ell_2,c} = C_{\ell_1\ell_2} \left[\bigoplus_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2} F_{\ell,c} \right]$
- Construct scalars: $\sum_m |[F_\ell]_m|^2$



Aggregation



Clebsch-Gordan aggregation:

$$F_i = \sum_{j \in N(j)} E_{ij} \otimes_{\text{CG}} F_j$$

→ Ensures covariance!



Table 1. GDB-9 results

	Cormorant	SchNet [3]	NMP [4]	WaveScatt [5]
α (bohr ³)	0.085	0.235	0.092	0.160
$\Delta\epsilon$ (eV)	0.061	0.063	0.069	0.118
ϵ_{HOMO} (eV)	0.034	0.041	0.043	0.085
ϵ_{LUMO} (eV)	0.038	0.034	0.038	0.076
μ (D)	0.038	0.033	0.030	0.340
C_v (cal/mol K)	0.026	0.033	0.040	0.049
G (eV)	0.020	0.014	0.019	0.022
H (eV)	0.021	0.014	0.017	0.022
R^2 (bohr ²)	0.961	0.073	0.180	0.410
U (eV)	0.021	0.019	0.020	0.022
U_0 (eV)	0.022	0.014	0.020	0.022
ZPVE (meV)	2.027	1.700	1.500	2.000

Table 2. MD-17 results

	Cormorant	DeepMD [6]	DTNN [7]	SchNet [3]	GDML [2]	sGDML [8]
Aspirin	0.098	0.201	–	0.120	0.270	0.190
Benzene	0.023	0.065	0.040	0.070	0.070	0.100
Ethanol	0.027	0.055	–	0.050	0.150	0.070
Malonaldehyde	0.041	0.092	0.190	0.080	0.160	0.100
Naphthalene	0.029	0.095	–	0.110	0.120	0.120
Salicylic Acid	0.066	0.106	0.410	0.100	0.120	0.120
Toluene	0.034	0.085	0.180	0.090	0.120	0.100
Uracil	0.023	0.085	–	0.100	0.110	0.110

- [1] R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld. Scientific Data, 1, 140022 (2014).
- [2] S. Chmiela, A. Tkatchenko, H. E. Sauceda, I. Poltavsky, K. T. Schütt, and K.-R. Müller. Sci. Adv. 3, e1603015 (2017)
- [3] K. T. Schütt, H. E. Sauceda, P.-J. Kindermans, A. Tkatchenko, and K.-R. Müller. J. Chem. Phys. 148, 241722 (2018)
- [4] J. Gilmer, S. S. Schoenholz, P. F. Riley, O. Vinyals, and H. E. Dahl. PMLR 70, 1263, (2017).
- [5] M. Hirn, S. Mallat, and N. Poilvert. Multiscale Modeling Simulation, 15, 827 (2017).
- [6] L. Zhang, J. Han, H. Wang, R. Car, and W. E. Phys. Rev. Lett., 120, 143001 (2018).
- [7] K. T. Schütt, F. Arbabzadah, S. Chmiela, K.-R. Müller, and A. Tkatchenko. Nat. Comm. 8, 13890 (2017).
- [8] S. Chmiela, H. E. Sauceda, K.-R. Müller, and A. Tkatchenko. Nat. Comm., 9, 3887 (2018).

