Cormorant: COvaRiant MOleculaR Artificial Neural neTworks

Spotlight Presentation

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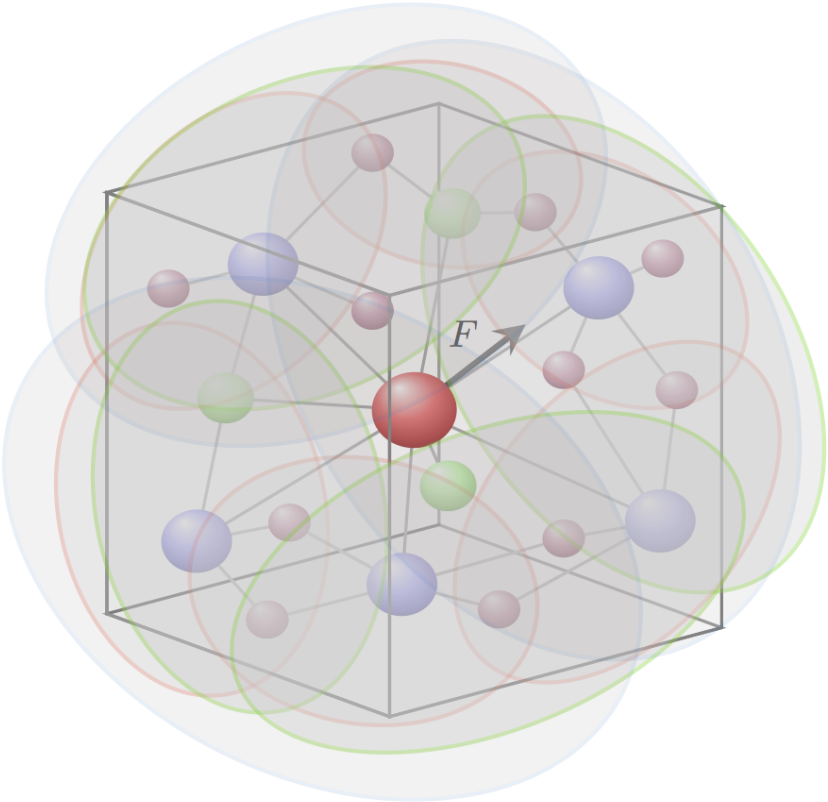
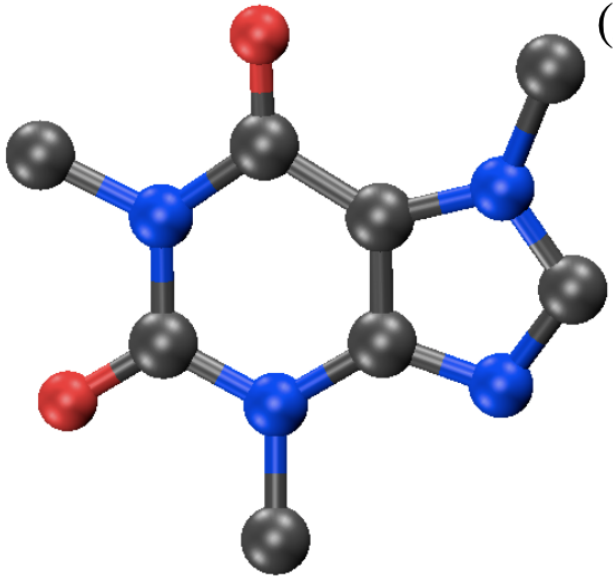
Learning on molecular data



$$F(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_m)$$

Learn on molecules:

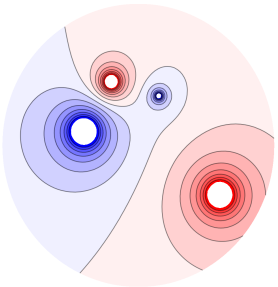


Data has built-in symmetry

! Use covariant activations!

The multipole expansion

$$\sum_i Z_i = j\mathbf{r} \quad \mathbf{r}_i j = \quad Q_0 Y^0(\hat{\mathbf{r}}) = r + \quad Q_1 Y^1(\hat{\mathbf{r}}) = r^2 + \quad Q_2 Y^2(\hat{\mathbf{r}}) = r^3 + \cdots$$



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":
$Q_{\grave{}} \; ! \quad D_{\grave{}}(R)Q_{\grave{}}$

Clebsch-Gordan Transformation

Group theory:

$$D^{\ell_1}(R) \quad D^{\ell_2}(R) = C^{\dagger}_{\ell_1,\ell_2} \sum_{\ell=|\ell_1-\ell_2|}^{M=\ell_1+\ell_2} D^{\ell}(R) \; C_{\ell_1,\ell_2}$$

$D^{\ell}(R)$: Wigner-D (Rotation) matrix
$C_{\ell_1\ell_2}$: Clebsch-Gordan matrix
$R \in SO(3)$

SO(3)-Vectors

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

Transforms covariantly: $F_{\ell;c} \to D^{\ell}(R) F_{\ell;c}$

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Linearly mixed: $\sum_{c} F_{\ell;c'} W_{c'c}$

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Clebsch-Gordan product: $F_{\ell_1;c} \otimes_{CG} F_{\ell_2;c} = C_{\ell_1 \ell_2} \bigoplus_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2} F_{\ell;c}$

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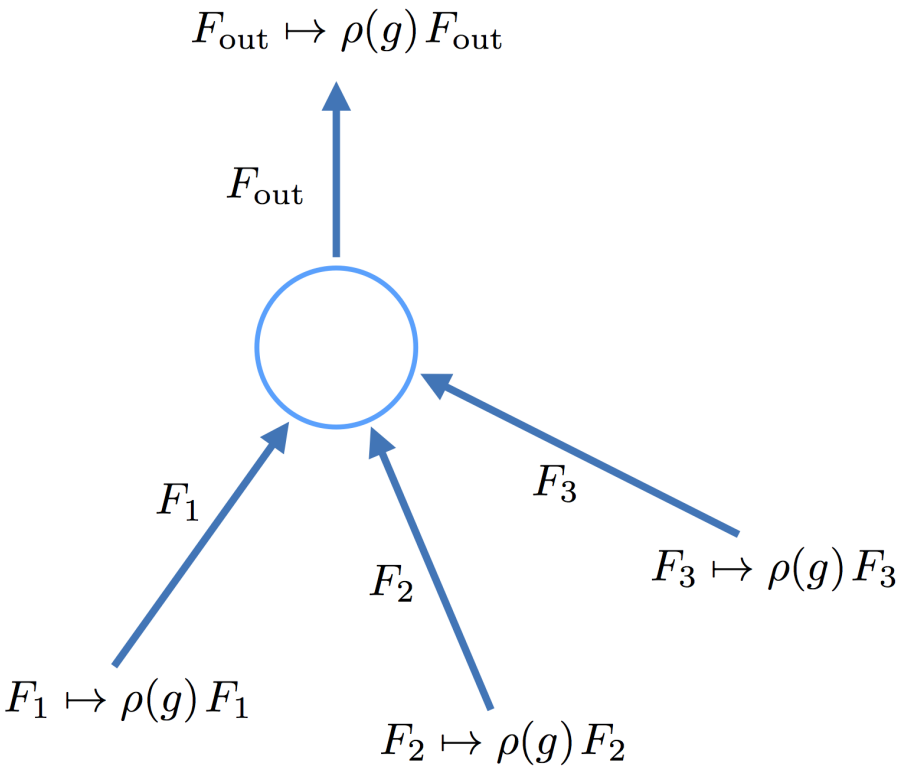
Construct scalars: $\sum_{m} |[F_{\ell}]_m|^2$

Aggregation



Clebsch-Gordan aggregation:

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

! Ensures covariance!

Experiments

Table 1. GDB-9 results

	Cormorant	SchNet [3]	NMP [4]	WaveScatt [5]
(bohr^3)	**0.085**	0.235	0.092	0.160
Δ (eV)	**0.061**	**0.063**	0.069	0.118
HOMO (eV)	**0.034**	0.041	0.043	0.085
LUMO (eV)	**0.038**	**0.034**	**0.038**	0.076
(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

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[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. Muller, and A. Tkatchenko. Nat. Comm. 8, 13890 (2017).
[8] S. Chmiela, H. E. Sauceda, K.-R. Muller, and A. Tkatchenko. Nat. Comm., 9, 3887 (2018).