# Lecture 26: Physics-informed deep neural networks

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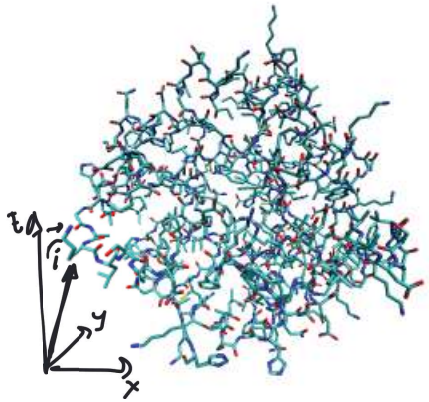
## Symmetries, invariance, and equivariance

# Example: Energy symmetries of a protein molecule

$\underline{R} = (\vec{r}_1, \dots, \vec{r}_N)$

$T_1 \qquad T_N$ : types of atom




https://upload.wikimedia.org/wikipedia/commons/6/6e/Proteinviews-1tim.png

**Energy**: $E(\underline{R})$ = Quantum mechanics (DFT)

**Problem**: Learn $E(\underline{R})$ with a finite number of simulations. $(\underline{R}_i, F_i)$.

$\dim(\underline{R}) = 3N$, $N = 200 \to 600$.

**Symmetries**:

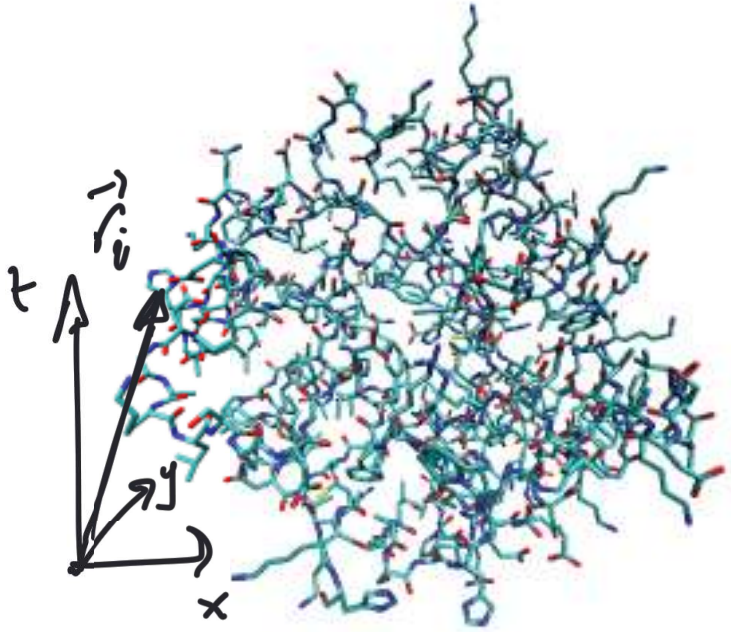
- $Q$ rotations: $E(Q\underline{R}) = E(Q\underline{r}_1, \dots, Q\underline{r}_N) = E(\underline{R})$ (invariant)
- $T$ translations: $E(T\underline{R}) = E(\underline{R})$ (invariant)
- $\pi$ permutation of same atom

$$E(\underset{C}{\underline{r}_1}, \underset{C}{\underline{r}_2}, \underset{C}{\underline{r}_3}, \dots) = E(\underset{C}{\underline{r}_2}, \underset{C}{\underline{r}_1}, \underset{C}{\underline{r}_3}, \dots) = E(\underset{C}{\underline{r}_3}, \underset{C}{\underline{r}_1}, \underset{C}{\underline{r}_2}, \dots)$$

$$E(\pi\underline{R}) = E(\underline{R})$$

Can you build these invariance in a DNN?

# Example: Force symmetries of a protein molecule

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$$\underline{F}(\underline{R}) = -\nabla_{\underline{R}} E(\underline{R})$$

$$(\underline{R}_i, \underline{F}_i)$$

- $\underline{F}(T\underline{R}) = \underline{F}(\underline{R})$ (invariance)
- $\underline{F}(\pi\underline{R}) = \pi\underline{F}(R)$ (equivariance)
- $\underline{F}(Q\underline{R}) = Q^{*}\underline{F}(\underline{R})$ (covariance)

How to encode in DNN?

# Encoding symmetries, invariance, and equivariance

- Open research
- Some promising work:
  - Thiede, E. H.; Hy, T. S.; Kondor, R. The General Theory of Permutation Equivarant Neural Networks and Higher Order Graph Variational Encoders. *arXiv:2004.03990 [cs, stat]* **2020**.