CS 6824:
Geometric Deep Learning for Molecular Representation

Acknowledgement:
Many of the images in the slides are derived from images.google.com or other publicly available sources.

"In the field of deep learning we have this 'zoo' of different neural network architectures. It is often hard to see the relationship between different methods because so many things are being reinvented and rebranded." — Michael Bronstein

ICLR 2021 Keynote

https://www.youtube.com/watch?v=w6Pw4MOzMuo

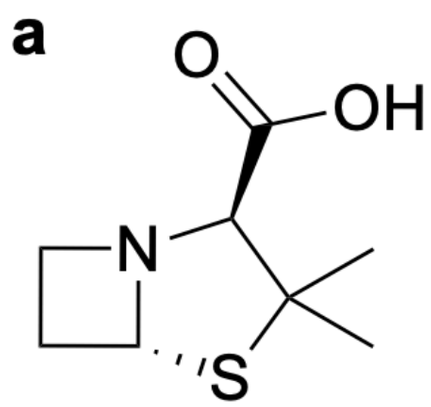
“Geometric Deep Learning: The Erlangen Programme of ML"

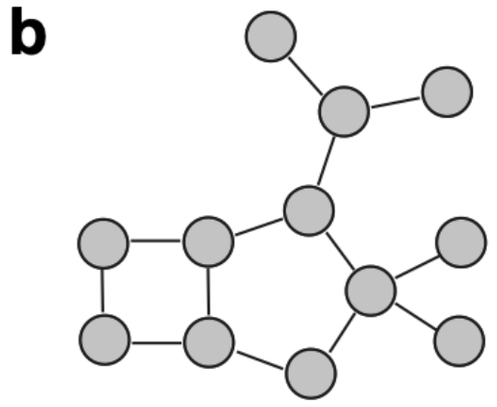
by

Michael Bronstein

The International Conference on Learning Representations (ICLR)

Molecular representation





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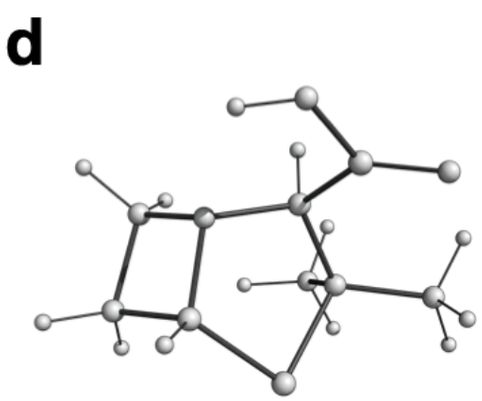

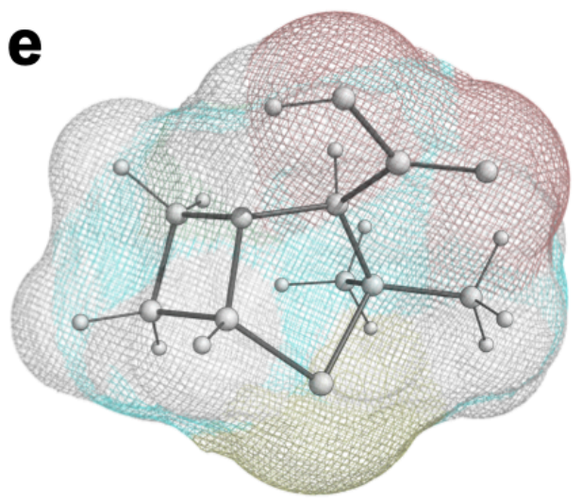

https://arxiv.org/pdf/2107.12375.pdf

Geometric deep learning for molecules

Table 1: *Summary of selected geometric deep learning (GDL) approaches for molecular modeling.* For each approach, the utilized molecular representation(s) and selected applications are reported. 1D, one-dimensional; 2D, two-dimensional; 3D, three-dimensional.

GDL approach	**Molecular representation(s)**	**Applications**
Graph neural networks (GNNs)	2D and 3D molecular graph, and 3D point cloud.	Molecular property prediction in drug discovery [37, 38] and in quantum chemistry for energies [39–41], forces [41–43] and wavefunctions [44], CASP [45, 46], and generative molecular design [47, 48].
3D convolutional neural networks (3D CNNs)	3D grid.	Structure-based drug design and property prediction [49, 50].
Mesh convolutional neural networks (geodesic CNNs or 3D GNNs)	Surface (mesh) encoded as a 2D grid or 3D graph.	Protein-protein interaction prediction and ligand-pocket fingerprinting [18].
Recurrent neural networks (RNNs)	String notation (1D grid).	Generative molecular design [19, 51], synthesis planning [52], protein structure prediction [53] and prediction of properties in drug discovery [54, 55].
Transformers	String notation encoded as a graph.	Synthesis planning [56], prediction of reaction yields [57], generative molecular design [58], prediction of properties in drug discovery [59], and protein structure prediction [6, 7].

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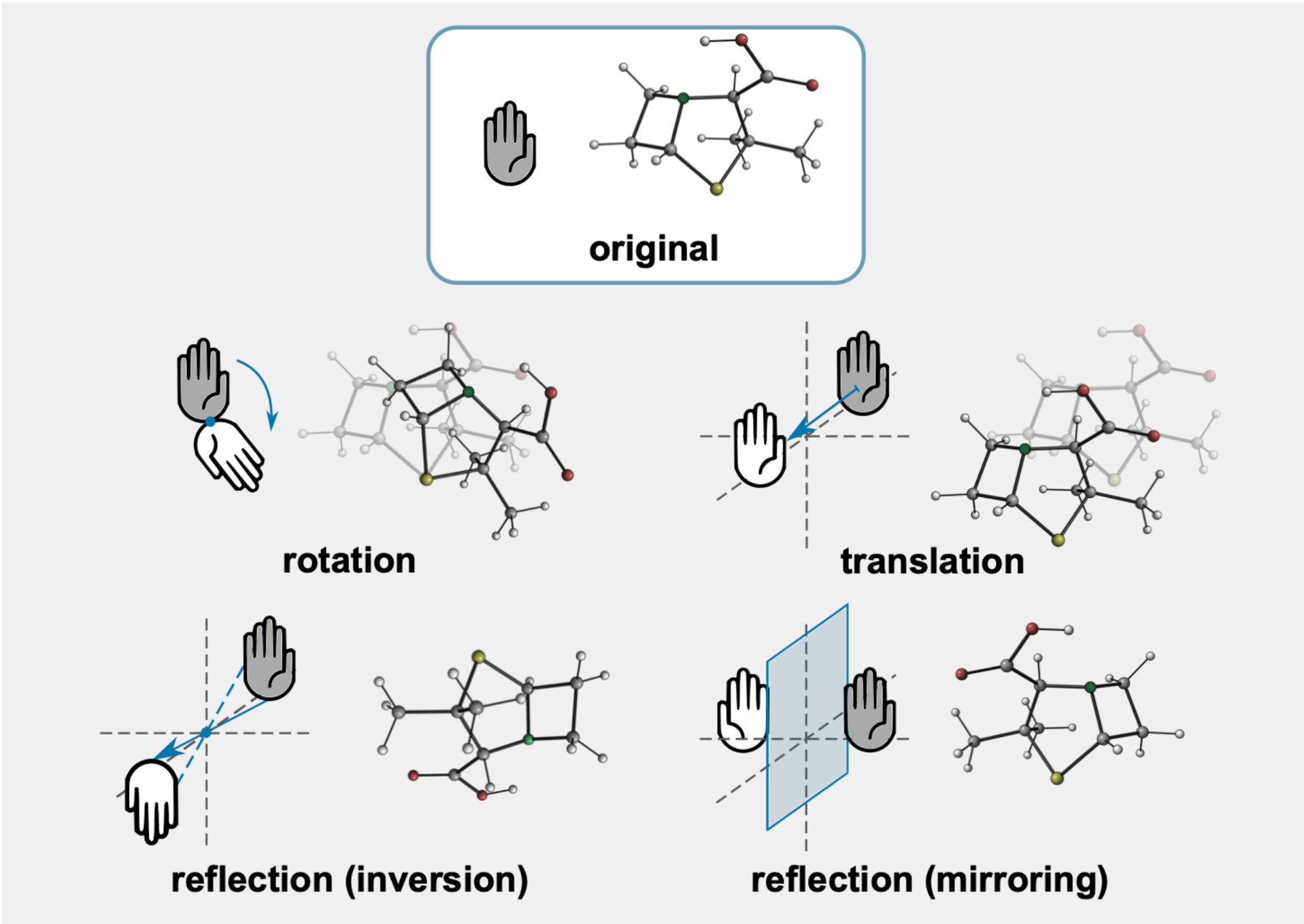
Euclidean symmetries in molecular systems



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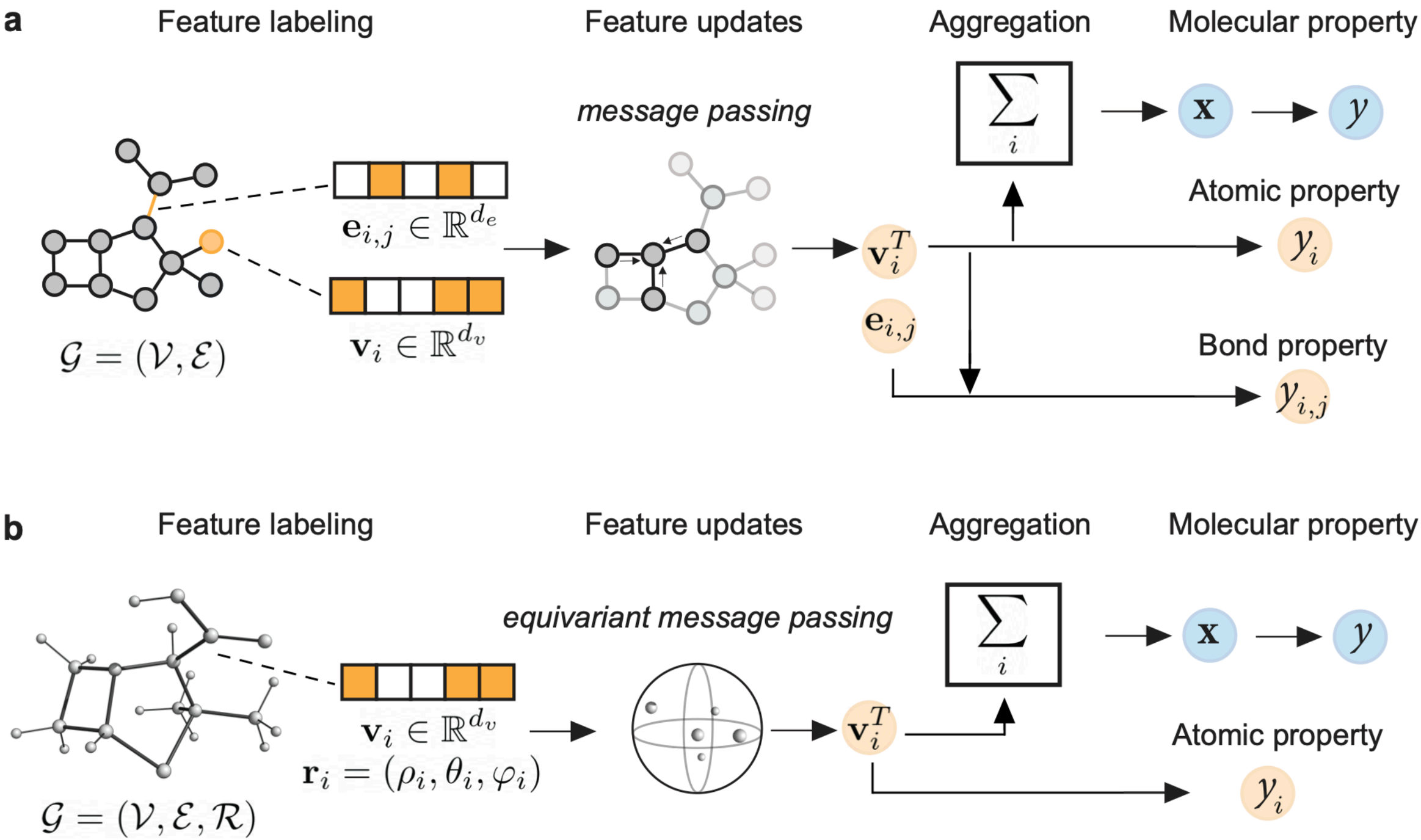
Deep learning on molecular graphs



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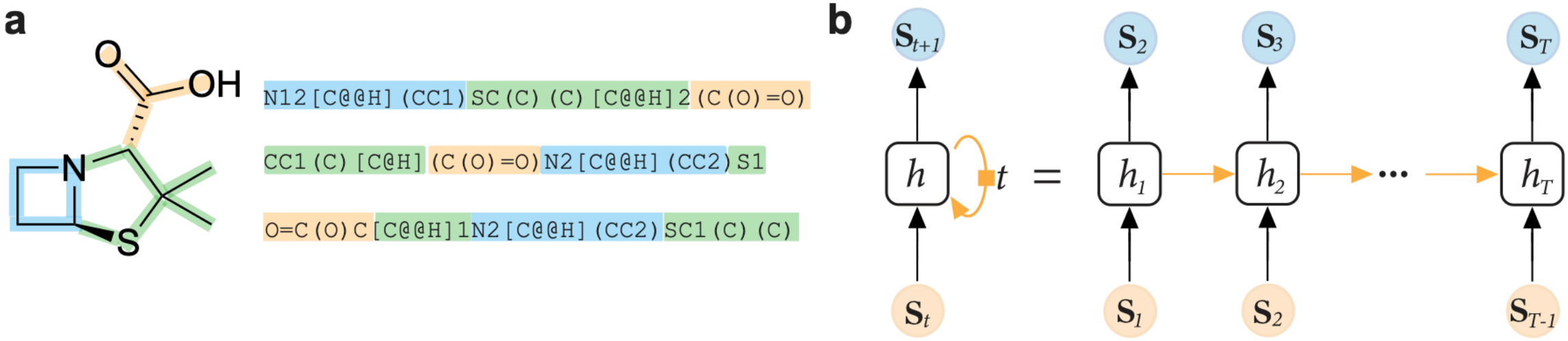
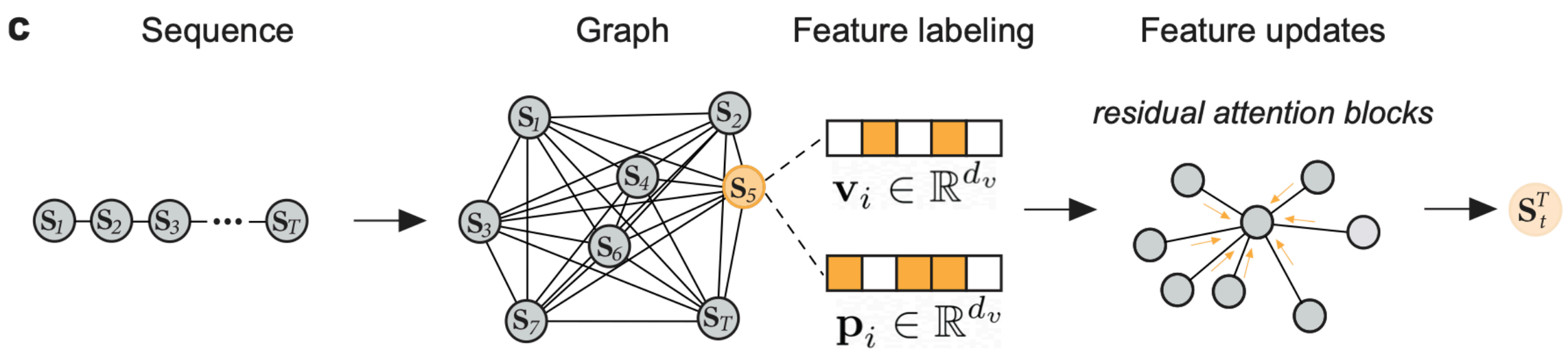
Chemical language models





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