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Examples of Machine Learning to Process and Model Large Datasets

Big Data and Machine Learning for Clean Coal and Carbon Management Strategic Planning Workshop

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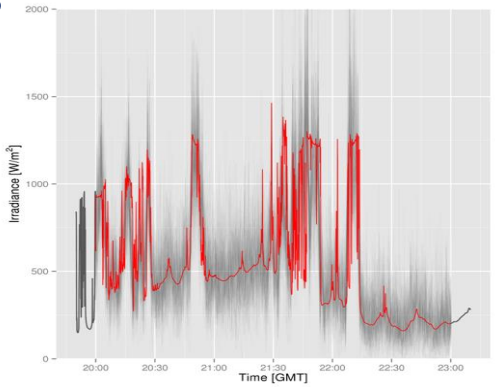
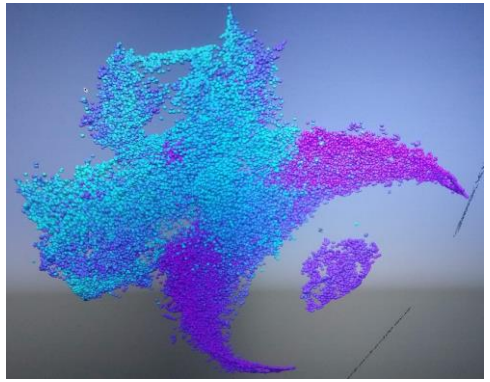
Machine-learning and statistical techniques enable cleansing, discovery, and modeling of massive datasets.

- Anomaly-detection and imputation methods automate the cleansing of large datasets.



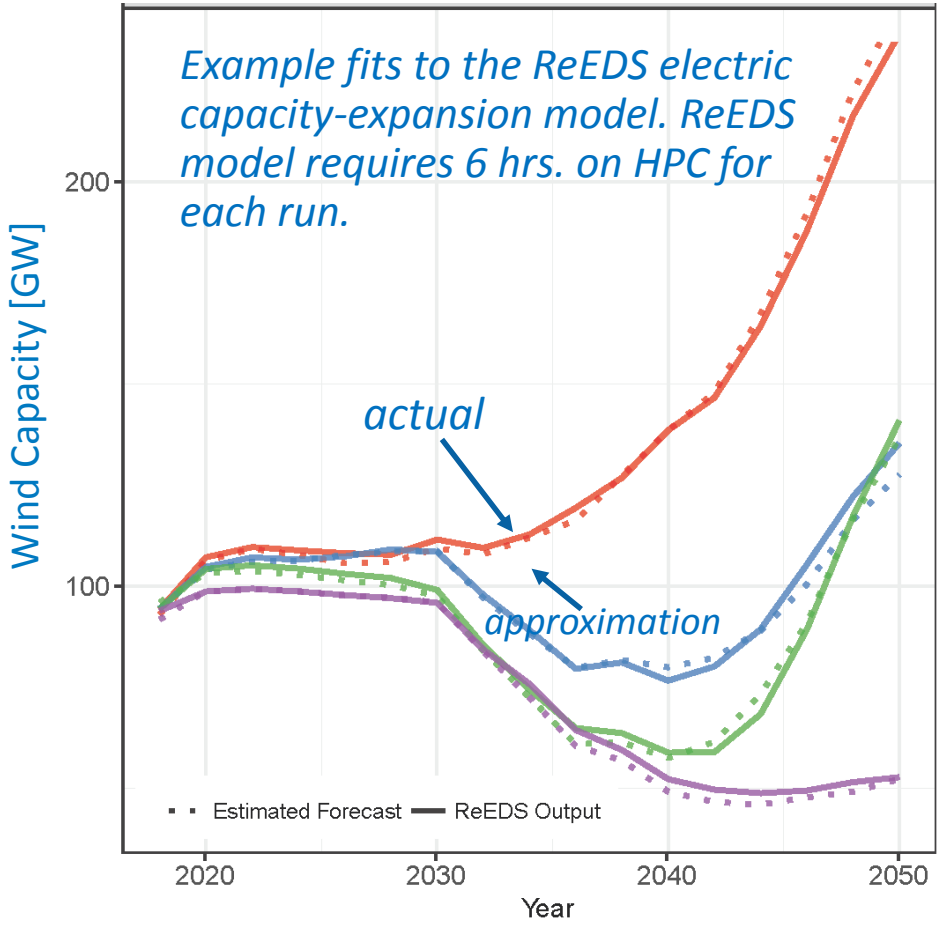
Reconstruction (black) of missing solar irradiance data (red) using a wavelet-based multi-scale covariance model.

- Dimension-reduction techniques and self-organized maps identify insightful patterns and low-dimensional features embedded in big datasets.



Abstract 3D feature visualization of a 50-dimensional dataset of 1.8 million simulations of bioenergy industry scenarios.

- Deep neural networks provide fast, high-quality approximations to state-of-the-art energy simulations.



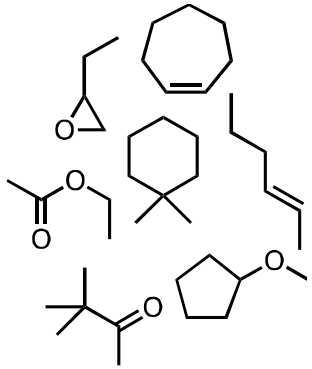
ReEDS: Regional Economic Development Scenario

Big Data is used to Train ANNs to Predict Material Properties from Molecular Structure

Accelerate the Design of performance-advantaged biomass-derived polymers

Explain novel behavior of bio-derived polymers seen in laboratory

Predict and Suggest new formulations for bio-derived polymers to synthesize in lab

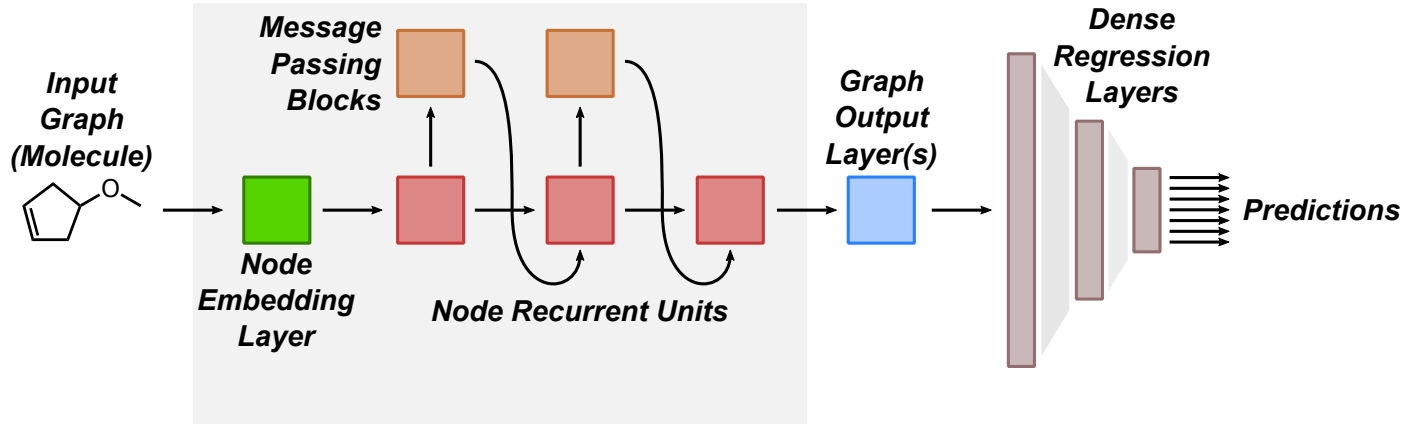


Traditional Quantitative Structure Property Relationship learning

Molecular Descriptors / Fingerprints → $\begin{pmatrix} u_1 \\ v_1 \\ w_1 \\ \vdots \\ u_n \\ v_n \\ w_n \end{pmatrix}$ → Traditional Machine Learning

End to end learning → **Property Prediction**

Single step from atomic structure to prediction.
Optimal molecular representation 'learned' from the data



Data
- Chemistry Molecular Databases
- Polymer Property Databases
- Molecular Dynamics and QM
- Experiments

Machine Learning
- Transfer Learning from any Chemical Database

Application of ANNs to Predict Orbital Energies in Organic Photovoltaic Solar Cells

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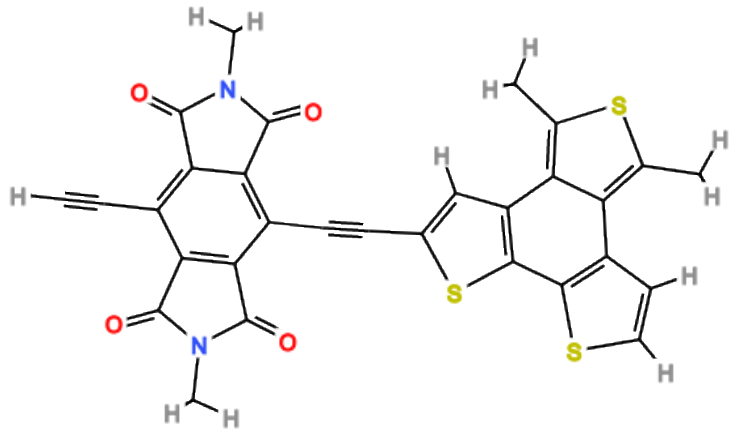
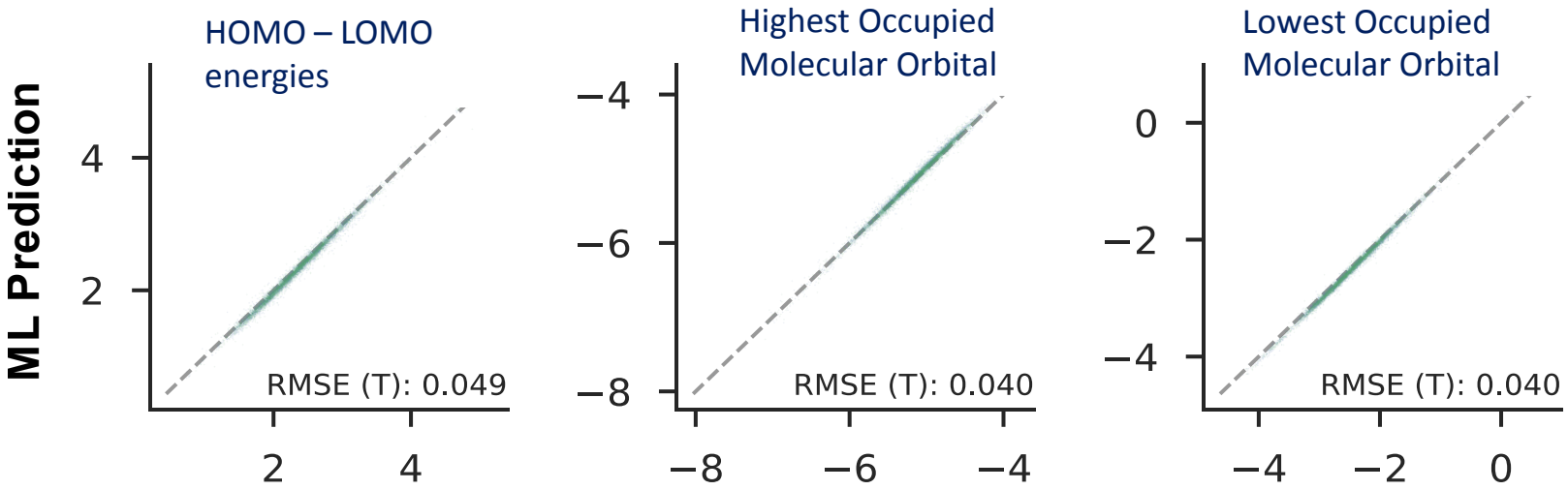
Computational Database for Active Layer Materials for Organic Photovoltaic Solar Cells



>90,000 monomers,
>50,000 with extrapolated polymer results



- Orbital energies predicted to ~1 kcal/mol (approximately experimental error)
- Computation times reduced by ~6 orders of magnitude: 10^{-3} s for ML, 10^{3} s for DFT

DFT, Density Functional Theory', is the numerically intensive computational result which is predicted with machine learning.

units in eV

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