Example projects

- Studying accuracy and robustness of models using frames (conventions) vs. equivariance vs. traditional (non-equivariant)
- Using learning objectives in 6.S966 to apply to other <u>algebraic structures</u> or projections
- ...

Disclaimer: there are tons of papers in this area -- this is not an exhaustive list!

See also https://github.com/Chen-Cai-OSU/awesome-equivariant-network

Pagent papers are at the outting edge: papers released a few years age are more for

Recent papers are at the cutting edge; papers released a few years ago are more foundational **Topics**:

- Architectures
 - Convolutional networks (in general)
 - Group Equivariant Convolutional Networks, 2016
 - On the Generalization of Equivariance and Convolution in Neural Networks to the Action of Compact Groups, 2018
 - Steerable networks
 - Steerable CNNs, 2016
 - 3D Steerable CNNs: Learning Rotationally Equivariant Features in Volumetric Data, 2018
 - General E(2) Equivariant Steerable CNNs, 2019
 - Spherical data
 - Spherical CNNs, 2018
 - Clebsch–Gordan Nets: a Fully Fourier Space Spherical Convolutional Neural Network, 2018
 - Graphical data
 - Provably Powerful Graph Networks, 2019
 - <u>Understanding and Extending Subgraph GNNs by Rethinking Their</u> Symmetries, 2022
 - Sign and Basis Invariant Networks for Spectral Graph Representation Learning, 2022
 - Complete Neural Networks for Euclidean Graphs, 2023
 - Set data / other permutational symmetries
 - Deep Sets, 2018
 - On Learning Sets of Symmetric Elements, 2020
 - Point cloud and geometric graph data
 - Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds, 2018
 - Vector Neurons: A General Framework for SO(3)-Equivariant Networks,
 2021
 - <u>SE(3)-Transformers: 3D Roto-Translation Equivariant Attention Networks</u>, 2020
 - Geometric and Physical Quantities Improve E(3) Equivariant Message Passing, 2022
 - Lie groups

- Generalizing Convolutional Neural Networks for Equivariance to Lie Groups on Arbitrary Continuous Data, 2020
- A General Theory of Equivariant CNNs on Homogeneous Spaces, 2020
- A Practical Method for Constructing Equivariant Multilayer Perceptrons for Arbitrary Matrix Groups, 2021

Theoretical properties

- Universality and function approximation
 - Universal approximations of invariant maps by neural networks, 2018
 - Graph neural networks
 - On the Universality of Invariant Networks, 2019
 - Universal Invariant and Equivariant Graph Neural Networks, 2019
 - Scalars are universal: Equivariant machine learning, structured like classical physics, 2023
 - On the Universality of Rotation Equivariant Point Cloud Networks, 2020
 - Exponential Separations in Symmetric Neural Networks, 2022
- Sample complexity and generalization
 - Provably Strict Generalisation Benefit for Equivariant Models, 2021
 - Learning with invariances in random features and kernel models, 2021
 - An Analysis of the Effect of Invariance on Generalization in Neural Networks, 2019
 - <u>Understanding the Generalization Benefit of Model Invariance from a</u>
 Data Perspective, 2021
 - On the Sample Complexity of Learning under Invariance and Geometric Stability, 2021
 - A PAC-Bayesian Generalization Bound for Equivariant Networks, 2022
- Optimization
 - Implicit Bias of Linear Equivariant Networks, 2022
 - On the Implicit Bias of Linear Equivariant Steerable Networks: Margin, Generalization, and Their Equivalence to Data Augmentation, 2023
- Approximate symmetries
 - o Residual Pathway Priors for Soft Equivariance Constraints, 2021
 - Approximately Equivariant Networks for Imperfectly Symmetric Dynamics, 2022.
 - A General Theory of Correct, Incorrect, and Extrinsic Equivariance, 2023
 - Breaking symmetries
 - Finding symmetry breaking order parameters with Euclidean neural networks, 2021
 - Breaking the Symmetry: Resolving Symmetry Ambiguities in Equivariant Neural Networks. 2022
 - Discovering Symmetry Breaking in Physical Systems 2024
 - Symmetry Breaking Sets 2023
- Learning symmetries
 - Meta-Learning Symmetries by Reparameterization, 2021
 - Automatic Symmetry Discovery with Lie Algebra Convolutional Network, 2021
 - <u>Learning Invariances in Neural Networks, 2020</u>
 - <u>Discovering Symmetry Group Structures via Implicit Orthogonality Bias 2024</u>

- Equivariant reinforcement learning
 - o SO(2) -Equivariant Reinforcement Learning, 2022
 - MDP Homomorphic Networks: Group Symmetries in Reinforcement Learning,
 2020
- Equivariant self-supervised learning
 - Robust Self-Supervised Learning with Lie Groups, 2022
 - Equivariant Contrastive Learning, 2022
- Equivariant generative models
 - Equivariant Flows: Exact Likelihood Generative Learning for Symmetric Densities, 2020
 - E(n) Equivariant Normalizing Flows, 2022
 - Symphony: Symmetry-Equivariant Point-Centered Spherical Harmonics for Molecule Generation 2024
 - Ophiuchus: Scalable Modeling of Protein Structures through Hierarchical Coarse-graining SO(3)-Equivariant Autoencoders, 2023
 - o MatterGen: a generative model for inorganic materials design 2023
- Equivariant autoencoders
 - Unsupervised Learning of Group Invariant and Equivariant Representations
- Encoding symmetries in latent spaces
 - Structuring Representations Using Group Invariants, 2022
 - o Cross-Domain 3D Equivariant Image Embeddings, 2019
 - Learning Symmetric Embeddings for Equivariant World Models, 2022
- Non-architectural approaches to equivariance
 - Data augmentation
 - A Group-Theoretic Framework for Data Augmentation, 2019
 - Frames
 - Frame Averaging for Invariant and Equivariant Network Design, 2021
 - Separators
 - Low Dimensional Invariant Embeddings for Universal Geometric Learning, 2022
 - Group-invariant max filtering, 2022
 - Equivariance with Learned Canonicalization Functions, 2023
- Symmetries in learning algorithms
 - Why Are Convolutional Nets More Sample Efficient than Fully-Connected Nets?,
 2021
 - o On the non-universality of deep learning: quantifying the cost of symmetry, 2022
- Symmetries of neural networks
 - Equivariant Architectures for Learning in Deep Weight Spaces, 2023
 - Permutation Equivariant Neural Functionals, 2023
- Gauge equivariance
 - o Gauge Equivariant Convolutional Networks and the Icosahedral CNN, 2019
- Miscellaneous
 - The Lie Derivative for Measuring Learned Equivariance, 2022
- Applications (just a few samples -- this is by no means an exhaustive list!)
 - Drug discovery / biology

- Equivariant Diffusion for Molecule Generation in 3D, 2022
- DiffDock: Diffusion Steps, Twists, and Turns for Molecular Docking, 2023
- Chemistry / materials / molecular dynamics
 - Cormorant: Covariant Molecular Neural Networks, 2019
 - MACE: Higher Order Equivariant Message Passing Neural Networks for Fast and Accurate Force Fields, 2023
 - <u>E(3)-Equivariant Graph Neural Networks for Data-Efficient and Accurate Interatomic Potentials</u>, 2021
 - Equiformer: Equivariant Graph Attention Transformer for 3D Atomistic Graphs, 2023
 - Spherical Channels for Modeling Atomic Interactions, 2022
 - EquiformerV2: Improved Equivariant Transformer for Scaling to Higher-Degree Representations
- o PDEs and dynamics
 - Incorporating Symmetry into Deep Dynamics Models for Improved Generalization, 2020
 - Lie Point Symmetry Data Augmentation for Neural PDE Solvers, 2022
- Astronomy
 - <u>Translation and Rotation Equivariant Normalizing Flow (TRENF) for Optimal Cosmological Analysis</u>. 2022
- Physics
 - Lorentz Group Equivariant Neural Network for Particle Physics, 2020
 - Equivariant Flow-Based Sampling for Lattice Gauge Theory, 2020
- Robotics
 - Edge Grasp Network: A Graph-Based SE(3)-invariant Approach to Grasp Detection, 2022
- Vision
 - Equivariant Multi-View Networks, 2019 (see also Kostas Daniilidis and Leonidas Guibas' labs' work more generally)