Lie Groups with Applications to Machine Learning and Quantum Computing

Course Syllabus

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Contents

Course Material

- Hall, Brian C. *Lie Groups, Lie Algebras, and Representations.*
- Nielsen, Michael A., and Isaac L. Chuang. *Quantum Computation and Quantum Information.*
- Bronstein, Michael M. et al, “Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges.” *arXiv preprint* arXiv:2104.13478.
- Cohen, Taco, and Max Welling. “Group Equivariant Convolutional Networks.” *Proceedings of the 33rd International Conference on Machine Learning* (ICML), 2016.

1 Introduction to Lie Groups

1.1 Basic Notions

- Review of Groups and Smooth Manifolds. Topological Groups.
  - Basic definitions and examples
  - Importance in mathematics and physics
- Definition of Lie Groups
  - Groups that are also smooth manifolds
  - Smooth group operations

1.2 Fundamental Examples

- Real Matrix Groups
  - General Linear Group $GL(n, \mathbb{R})$. Open subset of $\mathbb{R}^{n^2}$
  - Special Linear Group $SL(n, \mathbb{R})$. Determinant 1 condition
  - Orthogonal Group $O(n)$. Preserves Euclidean inner product, compact but possibly disconnected
  - Special Orthogonal Group $SO(n)$. Connected component of $O(n)$, represents rotations of Euclidean space
- Complex Matrix Groups
  - Unitary Groups $U(n)$. Preserves Hermitian inner product
  - Special Unitary Group $SU(n)$. Important for QM, simply connected

1.3 Lie Subgroups, Homogeneous Spaces, and Continuous Symmetries

- Lie Subgroups
  - Embedded subgroups, regular subgroups, closed subgroups
  - Examples: torus in $SU(n)$ (diagonal matrices w/ unit complex entries), $SO(n) \subset SU(n)$ (real rotations inside complex rotations), Parabolic subgroups, maximal tori
- Homogeneous Spaces
  - manifolds of the form $M = G/H$, where $H \subset G$ is closed subgroup and G is Lie
  - Examples: spheres, projective spaces, Grassmannians, flag manifolds
- Continuous Symmetries
  - Noether's theorem (first pass): every continuous symmetry corresponds to a conserved quantity
  - Examples: translation (momentum conservation), rotation (angular momentum conservation), phase transformation (charge conservation)

Reference

Hall, Chapter 1.

2 Lie Algebras and the Exponential Map

2.1 Lie Algebras

- Tangent space at the identity, left-invariant vector fields, derivations of smooth functions
- Lie bracket, main properties (anti-symmetric, Jacobi identity)
- Structure constants

2.2 Matrix Lie Algebras

- $\mathfrak{gl}(n, \mathbb{R})$: all $n \times n$ matrices
- $\mathfrak{sl}(n, \mathbb{R})$: trace zero matrices
- $\mathfrak{so}(n)$: skew-symmetric matrices
- $\mathfrak{u}(n)$: skew-Hermitian matrices

2.3 The Exponential Map

- Matrix Exponential
  - Power series definition
  - Convergence properties, computational methods
- One-Parameter Subgroups
  - of the form $\exp(tX)$ for $t \in \mathbb{R}$
  - geometric interpretation

2.4 Baker-Campbell-Hausdorff Formula

- Theorem statement. How do you solve for Z in the equation $e^X e^Y = e^Z$?
- First few terms, $Z = X + Y + \frac{1}{2}[X, Y] + \cdots$
- Applications

Reference

Hall, Chapters 2-3.

3 Representation Theory of Lie Groups and Lie Algebras

3.1 Representations

- Group Representations: homomorphisms $\rho : G \to GL(V)$
  - V is vector space (usually complex)
  - ρ preserves the group operation
- Lie Algebra Representations: linear maps $\varphi : \mathfrak{g} \to \mathfrak{gl}(V)$
  - φ preserves the Lie bracket
  - Connected to group representation via exponential map
  - Derived representations

3.2 Representation Theory of $SU(2)$

- Fundamental representation (2×2 matrices)
- Connection to angular momentum
- Pauli matrices as generators
- Brief discussion of weights

3.3 Peter–Weyl Theorem

- Motivation: generalizing Fourier series concept to more general compact groups than S^1
- Takeaway: Complete reducibility of f.d. unitary representations of compact groups
- Applications to quantum mechanics

Reference

Hall, Chapters 4-5.

4 Lie Groups in Quantum Mechanics and Quantum Computing

4.1 Quantum Mechanics

- Symmetry in Quantum Mechanics
  - Conservation laws to focus on: charge, spin, color
  - Noether's theorem, revisited
- Unitary Groups in Quantum Systems
  - $U(1)$ and phase transformations.
    * Represents conservation of charge
    * Example: $\psi \to e^{i\theta}\psi$ where $\theta \in \mathbb{R}$
    * Generator: charge operator Q
  - $SU(2)$ and spin systems.
    * Represents rotational symmetry for spin-$\frac{1}{2}$ particles
    * Generated by Pauli matrices
    * Example: rotation of spin state $|\uparrow\rangle$ to $\alpha|\uparrow\rangle + \beta|\downarrow\rangle$
  - $SU(3)$: Strong interactions and Quantum Chromodynamics (QCD)
    * Represents quark flavor symmetries
    * Important in particle physics
    * Eightfold Way (Gell-Mann matrices)

4.2 Quantum Computing

- Quantum Gates as Lie Group Elements
  - Single-Qubit Operations. All single-qubit gates are elements of $SU(2)$ up to global phase. Common gates:

$$\text{Pauli-X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \in SU(2) \tag{1}$$

$$\text{Hadamard} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \in SU(2) \tag{2}$$

  - Multi-Qubit Operations
    * n-qubit gates live in $SU(2^n)$
    * CNOT gate as an element of $SU(4)$
    * Entangling operations require non-local Lie group elements
- Lie Algebras in Quantum Computing
  - Quantum control through Hamiltonian evolution
  - Time evolution operator: $U(t) = \exp(-iHt/\hbar)$
  - H is element of the Lie algebra $\mathfrak{u}(n)$
  - Control problem: reaching target unitary through available Hamiltonians

Reference

Nielsen-Chuang, Chapters 1.3 and Chapter 7 (on quantum gates).

5 Symmetry and Invariance in Machine Learning

5.1 Why use Lie Groups in ML?

- Role of Symmetry in Data and Models
  - Images (rotations, translations, scaling)
  - Point clouds (rigid transformations)
  - Molecular structures (rotations, permutations)
- Benefits
  - Reduce sample complexity
  - Better generalization
  - Physics-informed models

5.2 Group Equivariant Convolutional Neural Networks

- Convolutional Neural Networks
  - Translation invariance
  - Extension to other symmetries
- Group Convolutional Neural Networks
  - Incorporating rotations and reflections
  - Mathematical formulation

5.3 Geometric Deep Learning Applications

- Molecular modeling
- Point cloud processing
- Robotic manipulation and computer vision

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- Bronstein, Michael M., *et al.* "Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges." *arXiv preprint* arXiv:2104.13478.
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6 Lie Groups and Equivariant Neural Networks

6.1 Equivariant Networks

- Mathematical Foundations
  - Lie groups acting on input and feature spaces
  - Equivariant maps and convolution
- Designing Neural Architectures with Lie Group Symmetries
  - Implementation strategies
  - Challenges and solutions

6.2 Continuous Symmetries in Data

- Applications to 3D data and point clouds
- Spherical CNNs and other specialized architectures

6.3 Physics-Informed Neural Networks

- Embedding physical laws into models
- Leveraging symmetries for better predictions

Reference

- Bronstein, Michael M., *et al.* “Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges.” *arXiv preprint* arXiv:2104.13478.
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7 Case Studies, Recent Research, and Future Directions

Topics

- Review of Key Concepts
  - Interconnections between Lie groups, ML, and QC
  - Recap of important results and theorems
- Case Studies
  - Recent papers applying Lie groups to ML and QC
  - Detailed analysis and discussion
- Open Problems and Research Directions
  - Potential areas for innovation
  - Interdisciplinary applications
- Discussion and Q&A
  - Addressing student questions
  - Encouraging further exploration

Fun Applications

Integrating Lie groups in cutting-edge ML architectures, advances in quantum hardware and software leveraging Lie theory.