Statistical Foundations of Invariance and Equivariance in Deep Artificial Neural Network Learning

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Overview

Review: Group representation theory

- Invariance and Equivariance: $\rho : G \to GL(V)$ is a group homomorphism $\rho(g_1 g_2) = \rho(g_1)\rho(g_2)$

  f is G- Invariant if $\quad f(\rho(\mathfrak{g})x) = f(x), \quad$ f is G- Equivariant if $\quad f(\rho(\mathfrak{g})x) = \rho(\mathfrak{g})f(x) \quad \forall \mathfrak{g} \in G$

  ▶ Invariance requires information *compression* quotienting out symmetries, equivariance means information is *transformed* consistently.
- Group actions (in statistical contexts):
  1. Acting on group elements, G on G
  2. Acting on (statistical) parameters in $\mathbb{R}^d$, i.e., $T_g x$ (V finite dimensional, $\rho(g)$ invertible matrices)
     - ▶ Example: 1D Location Scale family, $T_g : \theta \to \theta_g = a\theta + b$
  3. Acting on functions f (Left regular representations), i.e., $L_g f(g') = f(g^{-1}g'), f \in \mathbb{L}_2(G)$[1] ($V$ infinite)
     - ▶ Example: Acting on Statistical estimators, $L_g : \hat{\Theta} \to \hat{\Theta}$, $L_g \hat{\theta}(\theta \mid x) = \hat{\theta}(T_g^{-1}\theta \mid x), \theta \in \mathbb{R}^d$
- Example - Spatial Rotational symmetry: $SO(3) = \{R^T R = I, det(R) = 1, R \in \mathbb{R}^{3\times 3}\}$
  1. Matrix composing with matrix (matrix product) defines G acting on G
  2. Matrix ($R = T_g = \rho(g)$) acting on $\mathbb{R}^3$ is trivial. $GL(V) = GL(3, \mathbb{R}) \equiv \mathbb{R}^{3\times 3}$
  3. $SO(3)$ acting on estimators acts on the parameters inversely.

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[1] Can also be defined for other $\mathbb{L}_2$ spaces $L_g f(x) = f(T_g^{-1}x), f \in \mathbb{L}_2(\mathbb{R}^d), x \in \mathbb{R}^d$

Review: Deep Network Architecture

Two approaches to make deep network invariant/equivariant:

- Data Augmentation Limitation
- Architectural Design
  - $G-$invariant inference framework: several equivariant functions followed by a invariant layer.

Common architectural designs:

1. **MLP**: Universal function approximators, no symmetry built in, generalization contingent on training data distribution.
2. **CNN**: MLP with translational equivariance (segmentation)/invariance (classification). Equivariance realized via *translational weight sharing*.
3. **Discrete GCNN**: Data augmentation made implicit in the architectural design, discrete indexing g of the group G needed, *weight sharing across G*

$$f *_G K(g) = \sum_{h \in \mathbb{R}^n} f(h) K(T_g^{-1} h). \quad \text{Example: Scaling} : (f *_{\mathbb{R}_{>0}} K)(p, \lambda) = \sum_{q \in \mathbb{R}^2} f(p-q) K\left(\frac{1}{\lambda} q\right)$$

Review: Deep Network Architecture

4. **Steerable CNN**: Does not need group sampling (discrete indexing) schemes, Information stored as Fourier coefficients (Peter-Weyl Theorem for compact group G) [8]

$$\text{Forward}: \hat{f}(\rho_\ell) = [\mathcal{F}_G f]_\ell = \int_G f(g)\rho_\ell(g)dg, \text{Backward}: \left[\mathcal{F}_G^{-1}\hat{f}\right]_\ell = \sum_\ell d_{\rho_\ell} tr\left[\hat{f}(\rho_\ell)\rho_\ell(g^{-1})\right], \tag{1}$$

Steerable kernels satisfy kernel constraints: $K(hx) = \rho_{out}(h)K(x)\rho_{in}(h^{-1})$

- $SO(3)$ example: $K(x) = \sum_{\ell=0}^{L}\sum_{m=-\ell}^{\ell} c_m^\ell(\|x\|)Y_m^\ell\left(\frac{x}{\|x\|}\right)$,
- Equivariance: $Y_m^\ell(R(\theta,\phi)) = \rho^\ell(R)Y_m^\ell(\theta,\phi), (\theta,\phi)\in S^2, R\in SO(3), \rho^\ell\in\mathbb{R}^{(2\ell+1)\times(2\ell+1)}$ are the Wigner-D matrices. $\rho^\ell = [D_{-\ell}^\ell, ..., D_{-1}^\ell, D_0^\ell, ..., D_\ell^\ell]$, $[D_m^\ell(\cdot)]_{m'} : SO(3)\to\mathbb{R}$ is Wigner-D function.

5. **Seq to Seq Transformers**: Non-convolutional Approach, attention mechanism is permutation equivariant, unlike MLP the model weights are *feature dependent* $w(X)$
   - Properties: Scaling laws [6], In context learning functional regression problem [4].

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    - Review: Group (Representation) Theory, Deep Network Architectures
    - Relaxing the exact G-equivariant condition
    - Case Study: Group Invariance Case Study on Kreuzer Skarke Dataset
2. Statistical and Optimization practice under symmetry
    - Invariance, probabilistic symmetry and statistical inference
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Relaxing the equivariance constraint

Motivation: Material Impurity (Non-isotropicity for ∇^2), physical non-ideality factors

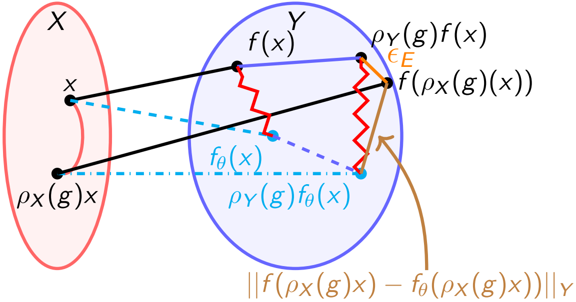
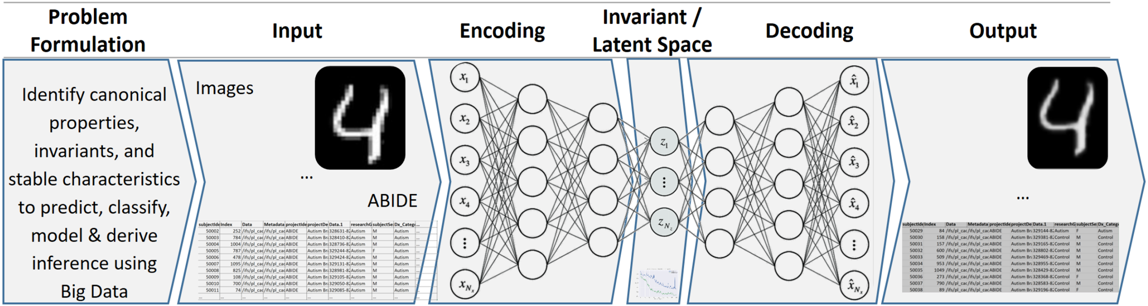


Figure: The problem with approximating an approximate G-equivariant function with G-equivariant function is that the two red zig zag lines cannot be simultaneously small. The solid lines stand for connections from G-equivariant (f_θ) inference. The dashed lines represent approximate G-equivariant (f) inferences.

- Approximate Equivariance[7]/Invariance :
  ϵ-approximate G-equivariant: $\forall\ g \in G$ and $\forall\ x \in X$, $\|f(\rho_X(g)(x)) - \rho_Y(g)f(x)\| \leq \epsilon_E$
  ϵ-approximate G-invariant: $\forall\ g \in G$ and $\forall\ x \in X$, $\|f(\rho_X(g)(x)) - f(x)\| \leq \epsilon_I$
- Lower Bound Error for approximate equivariance inference with full equivariance parametrization[7]
  - f_θ denotes the NN based G-equivariant network and f be the approximate equivariant framework. Assuming the Lipschitz condition, $\|\rho_Y(g)f_\theta(x) - \rho_Y(g)f(x)\|_Y \leq \kappa\|f_\theta(x) - f(x)\|_Y$. Then, $\exists x$, $\|f_\theta(x) - f(x)\| \geq \frac{1}{1+\kappa}\epsilon_E$

Bridging Theory and Practice: Emergent approximate invariance

Approximate invariance can also emerge from noise and constraints (latent dimension).



Problem Formulation | **Input** | **Encoding** | **Invariant / Latent Space** | **Decoding** | **Output**

Identify canonical properties, invariants, and stable characteristics to predict, classify, model & derive inference using Big Data

Figure: A schematic of DL network auto-encoding-decoding of handwritten images and the large ABIDE dataset along with identification of DL invariants that capture the intrinsic properties of the training data. This VAE framework may be used to produce synthetic realizations resembling the original training data.

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Group Invariant Learning on Kreuzer Skarke Dataset

Work with Christian Ewert, Sumner Magruder, Vera Maiboroda, Pragya Singh, and Daniel Platt. [2]

- Problem: Regression $\mathbb{R}^{4\times 26} \to \mathbb{Z}_+$
  - Symmetry Group: $S_4 \times S_{26}$.
  - Cardinality: $4! \times 26! = 9.7 \times 10^{27}$

  Data Augmentation impossible Arch-review
- Models: CNN, Xgboost, Invariant MLP, (Vision) Transformer, PointNet++, MLP with invariant features
- Data Preprocessing: Original, Original (Random) Permuted, Preprocessed, Preprocessed Permuted
- Main Findings:
  1. Approximately Invariant models outperform fully invariant models
  2. Group Invariant Preprocessing improves performance
  3. Building group invariance improves performance

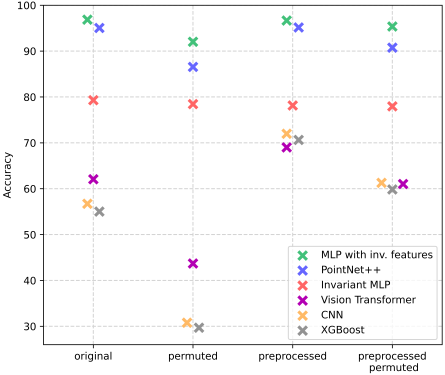

Figure: Different Architectures across group invariant preprocessing

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[2] `https://github.com/danielplatt/kreuzer-skarke-ML/blob/main/Group_Invariant_Kreuzer_Skarke.pdf`

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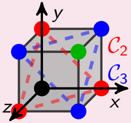
Invariance, probabilistic symmetry and statistical inference

Discrete Case



$\mathcal{C}_1 = \{(0,0,0)\}, S_{\mathcal{C}_1}(x) = 0$

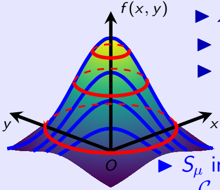
$\mathcal{C}_2 = \{(0,0,1),(0,1,0),(1,0,0)\}, S_{\mathcal{C}_2}(x) = 1$

$\mathcal{C}_3 = \{(0,1,1),(1,1,0),(1,0,1)\}, S_{\mathcal{C}_3}(x) = 2$

$\mathcal{C}_4 = \{(1,1,1)\}, S_{\mathcal{C}_4}(x) = 3$

- $X_1, X_2, X_3 \sim \text{Binomial}(\theta)$
- Sample space $\mathcal{X} = \{(x,y,z) \mid x,y,z \in \{0,1\}\}$
- (Minimal) Sufficient Statistic $S = x_1 + x_2 + x_3$
- $S(x)$ induced partition $\mathcal{X} = \mathcal{C}_1 \bigcup \mathcal{C}_2 \bigcup \mathcal{C}_3 \bigcup \mathcal{C}_4$

Continuous Case



- $X_1, X_2 \sim \mathcal{N}(\mu, \sigma^2)$
- Sample space: $\mathcal{X} = \mathbb{R}^2$
- (Minimal) sufficient statistics:

  Mean: $S_\mu = x_1 + x_2$

  Variance: $S_{\sigma^2} = x_1^2 + x_2^2$
- S_μ induced partition $\mathcal{X} = \bigcup_{t\in\mathbb{R}} \mathcal{C}_t$

  $\mathcal{C}_t = \{(x,y) \mid x + y = t\}$
- S_{σ^2} induce $\mathcal{X} = \bigcup_{t\in\mathbb{R}^+} \mathcal{C}_t$, $\mathcal{C}_t = \{(x,y) \mid x^2 + y^2 = t\}$

Figure: Discrete and continuous case of sample space partition induced by sufficient statistics. (Left): The sufficient statistic generates a partition of black, red, blue green dots. (Right): The sufficient statistic generates a partition of red isocontours for the variance and blue isocontours for the mean parameter.

- *Probabilistic Symmetry* is defined on random structures X_∞ (random variables, random graphs, random partitions,...). A random structure is *symmetric* to G if $g(X) \overset{d}{=} X, \forall X \in X_\infty, g \in G$. The canonical example being exchangeability [2].
- Sufficiency describe information relevant to inference, Invariance introduces irrelevance and needs to be quotient out.

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Metric Measure Symmetry & Measuring symmetry

Common symmetries in metric measures:

- Reparametrization symmetry.
  ▶ Physical properties (Curve length, Regional areas, Solid volumes) is independent of coordinate transformations.
  ▶ Canonical variable transform is coupled with a Jacobian term (r.v. Bivariate transform $f_{UV}(u, v) = f_{XY}(x(u, v), y(u, v))|J|$). When the $|J|$ factor is absorbed, the quantity is reparametrization invariant (Fisher information, Mutual information).
- Geometrical Transformation Symmetry
  ▶ Rotations (Cosine similarity, L2 logistic regression), Affine (Amari-Chentsov tensor[1])
- Problem specific symmetries:
  ▶ Optimal policy invariance under reward shaping $\tilde{R} = R + F(x, a, x') = R + \gamma\phi(x') - \phi(x)$: This non-classical invariance is generated from the Bellman objective function form.

Measuring Symmetry

One can use Lie derivative to quantify how much symmetry is aligned/violated (Locally) by rearranging the equivariance condition: [5]

$$\rho_{21}(g)[f](x) = \rho_2(g)^{-1} f(\rho_1(g))(x) \tag{2}$$

The Lie derivative generated by a vector field Y can be expanded using the rewritten condition

$$\mathcal{L}_Y(f) = \lim_{t\to 0} \frac{\rho_{21}(\phi_Y^t)[f] - f}{t} = \lim_{t\to 0} \frac{\psi^*_{exp(-tY)} \circ f \circ \psi_{exp(tY)} - f}{t} \tag{3}$$

- ϕ_Y^t is the local 1-parameter group generated by Y (flowing along the vector field Y with time t)
- $\psi_{exp(tY)} : \mathcal{M} \to \mathcal{M}$ is the manifold pushforward defined by the group action
- $\psi^*_{exp(-tY)} : T^*_{\phi_Y^t(p)}\mathcal{M} \to T^*_p\mathcal{M}$ is the pullback of the cotangent space. Namely, it pulls back the cotangent space at $\phi_Y^t(p)$ to p

Optimization Practice [3]

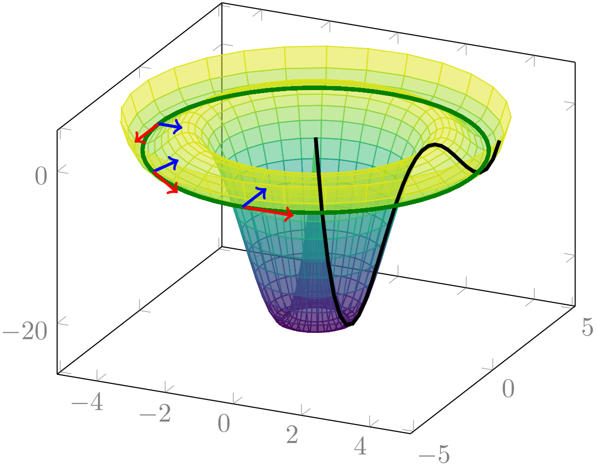


Figure: An illustration of a non-convex loss landscape with radial symmetry. $\mathcal{M}$: surface,$\mathcal{M}/G$: black curve

Symmetries on the functional landscape often entails non-convexity. In terms of optimizing on the total space $\mathcal{M}$ or quotient space $\mathcal{M}/G$

- For *first order* Riemannian gradient descent method, there is no difference utilizing the quotient structure or using the algorithm in the original space.
- For *second order methods*, Newton's method would be catastrophic for optimizing the loss in the original space $\mathcal{M}$, since Newton's method solves step direction in one shot.
- Using conjugate gradient to minimize the second order expansion mitigates the problem of solving an underdetermined system when optimizing in original space $\mathcal{M}$.

Overview

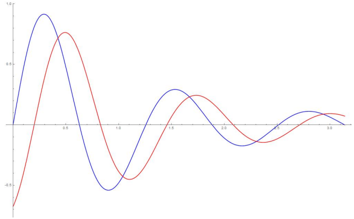
Biomedical Applications

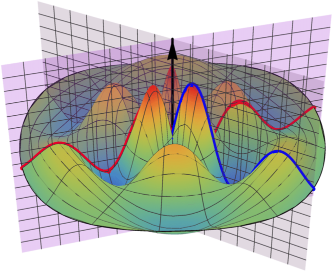
Biomedical Datasets demonstrate various classical and non-classical invariances

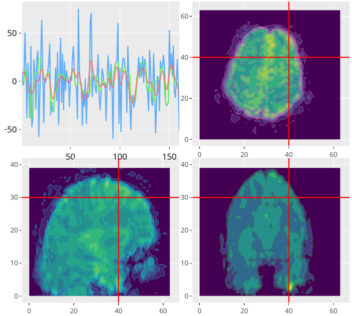
- Set data structure such as gene expression have permutation invariance
- Modeling Spatiotemporal measurements could be invariant to
    1. Spatial rotation, irrespective of the machine orientation selected (fMRI imaging, 2D pathology slices of 3D anatomy).
    2. Temporal translations. Same stimuli (Experimental condition) should give rise to same activation patterns across measurement taken times.

  ▶ More generally, this needs to be modeled as gauge invariance: Instrument changes may lead to measurement transformations (i.e., gauge transformations) tracking the same quantity between different devices, which subject to rigorous calibration is expected to yield stable inference, i.e., inference invariance/equivariance).
- fMRI preprocessing (e.g., registering the hypervolumetric data into a common 3D/4D spatiotemporal) atlas space to align the fMRI data and facilitate a form of inference invariance can be regarded as the "group invariant" preprocessing step.

Prospective study: Invariance, neuroimaging and spacekime analytics







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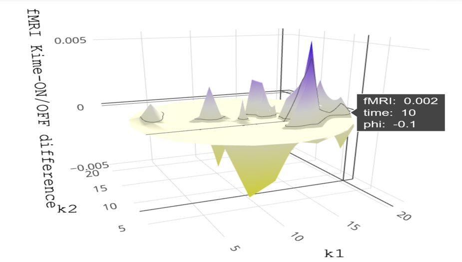

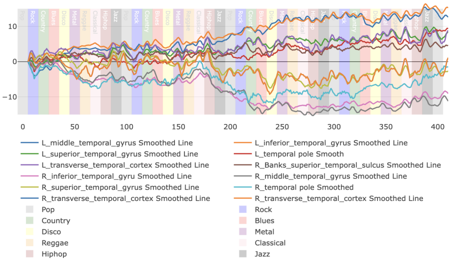

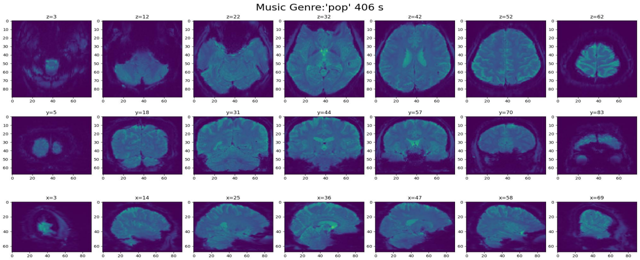

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