Learning Chern Numbers of Multiband Topological Insulators with Gauge Equivariant Neural Networks

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NEURAL INFORMATION PROCESSING SYSTEMS

Problem Setting

Topological Insulators

Topological Insulators: Materials that behave as insulators in their bulk but allow current to flow along their boundaries, due to underlying topological invariants (**Chern numbers**).

Tensor formulation

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- Chern Number: An integer $\tilde{C}$:

$$\tilde{C}\Big(\{W_k \,|\, k \in \Lambda\}\Big) = \frac{1}{2\pi} \sum_{k\in\Lambda} \operatorname{Im} \operatorname{Tr} \log W_k \,. \tag{1}$$

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- Gauge symmetry:

$$\tilde{C}\Big(\{W_k \,|\, k \in \Lambda\} \Big) = \tilde{C}\Big(\{\Omega_k^\dagger W_k \Omega_k \,|\, k \in \Lambda\} \Big) \quad \forall \{\Omega_k\}_{k\in\Lambda} \in \mathrm{U}(N)^{N_x \times N_y} \,. \tag{2}$$

Large Non-Abelian Gauge Symmetry

Gauge Symmetry

$$U_k^\mu \sim \Omega_k^\dagger U_k^\mu \Omega_{k+e_\mu}, \quad W_k \sim \Omega_k^\dagger W_k \Omega_k \tag{3}$$

- **Non-Commutative**: Unitary Matrix group.
- **Local**: One Unitary group at each grid point; traditional Lie group equivariance techniques (data augmentation, GCNN, etc.) fail.

GEBLNet: Local Gauge–Equivariant Network

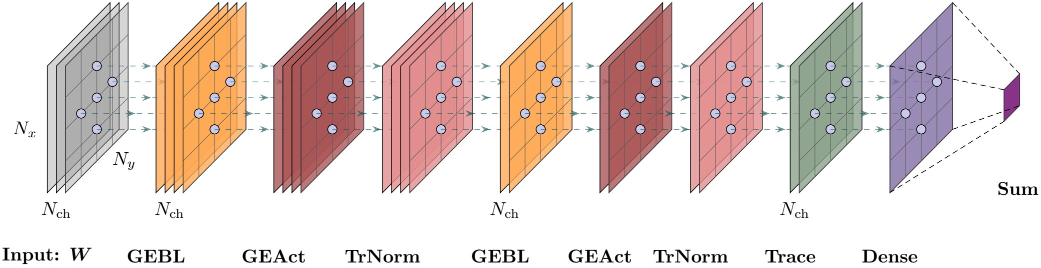

Figure: Architecture of GEBLNet [*Favoni et al. 2022*]. Each circle represents an independent grid point.

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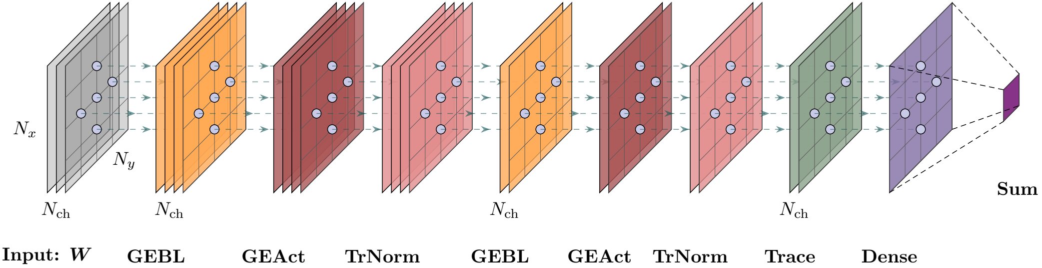

Figure: Architecture of GEBLNet [*Favoni et al. 2022*]. Each circle represents an independent grid point.

- **Purely local processing**: every point k is handled in isolation; no coupling between neighbours during feature extraction.
- **Gauge equivariance**: each layer manifestly preserves the gauge transformation and retains the matrix form outputs.

Implementation

- **Input:** $(W_k^\lambda) \in U(N)^{N_{\text{in}} \times N_{\text{site}}}$
- **Step 1:** Append identity matrix I to the input set
- **Step 2:**

$$W_k'^{\gamma} = \sum_{\mu,\nu} \alpha_{\gamma\mu\nu} \, W_k^\mu \, W_k^\nu$$

Intuition:

Constructs higher-order terms W^n from lower-order ones and form a polynomial.

Universal Approximation Theorem with GEBL

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Theorem (UAT for GEBLNet)

Let G be a compact Lie group. Assume the GEAct non-linearity is $\sigma = \tilde{\sigma} \circ \mathrm{Re}$ with $\tilde{\sigma}$ bounded and non-decreasing. Then GEBLNet can approximate any square-integrable conjugation invariant function $F \in L^2_{\text{class}}(G)$ to arbitrary accuracy.

Training Setup

Loss function

Given network output $f(W)$ and discrete Chern number $\tilde{C}$:

$$L_{\mathrm{g}} = \left\| f(W) - \tilde{C} \right\|_1, \qquad L_{\mathrm{std}} = \left\| \min\Big(\mathrm{std}\Big\{ g(W_k) \Big\}, \delta\Big) - \delta \right\|_1,$$

with $\delta = 0.5$.

$$\boxed{L_{\mathrm{total}} = L_{\mathrm{g}} + L_{\mathrm{std}}}$$

L_{std} prevents the network from collapsing to zero-outputs by enforcing point-to-point variation.

Model Capability Test: Band Number

Table: **Accuracy on a 5×5 grid.** GEBLNet is trained and evaluated for increasing band count N.

Bands N	4	5	6	7	8
Accuracy (%)	95.9	94.0	93.8	91.7	52.5

- High accuracy is retained up to $N = 7$ bands.

Training on Trivial Samples: Problem Statement

Setting

- Grid 5×5, $N = 4$ bands
- Only *topologically trivial* samples ($C = 0$)
- Need L_{std}

Result: GEBLNet without TrNorm fails

- Most seeds $\to$ outputs ≈ 0

Trace Explosion

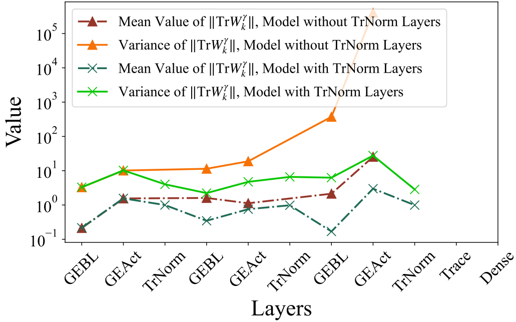


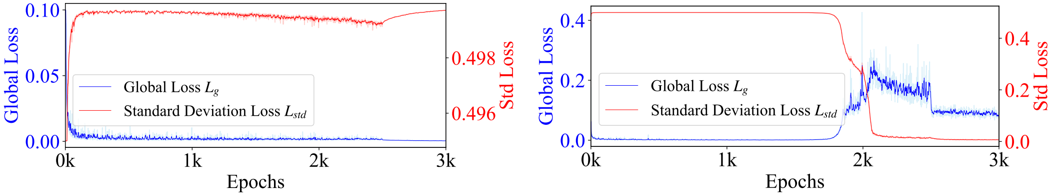
Figure: Statistics of trace per layer, with or without TrNorm

Trace Normalization (TrNorm)

$$W_k'^\gamma = \frac{W_k^\gamma}{\max(\varepsilon, \operatorname{mean}_\gamma\{|\operatorname{tr} W_k^\gamma|\})}$$

- Normalization over each channel so that $\operatorname{mean}_\gamma\{|\operatorname{tr} W_k^\gamma|\}$.
- Cancels trace explosion after every GEBL layer.

TrNorm Fixing the collision



Loss curves, seed 83. Left: no TrNorm (collapse). Right: with TrNorm (converges).

- **Turning point** (std. loss < 0.49) occurs between 1.3 k–1.9 k epochs for 4/5 seeds.
- Post-rescale accuracy on non-trivial data $92\% - 95\%$ (table below).

Generalization: Higher Dimensional Models

Higher Order Chern Number

For general $2M$ dimensional multiband system, the discretized Mth Chern number could be defined as

$$\tilde{C}_M = \frac{M!}{(2M)!(\pi i)^M} \sum_k \sum_{\mu_1,\ldots,\mu_{2M}} \mathrm{Tr}\epsilon_{\mu_1,\ldots,\mu_{2M}} \prod_{t=1}^{M} \log W_k^{\mu_{2t-1},\mu_{2t}}. \tag{4}$$

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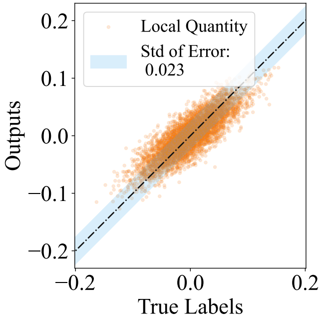
- For M=2 (four spatial dimensions) each point carries $\binom{4}{2} = 6$ loops (channels): $W_k^{\mu\nu}$.
- The approximation is not necessarily integer; evaluation metric is then mean absolute error (MAE), not exact accuracy.

Generalization: Higher Dimensional Models



Local quantity-truth comparison

- Points lie close to the line $y = x$: model reproduces the *local* topological quantity with high precision.
- Global MAE≈ 0.25: well within rounding error of the true second Chern number.

Generalization: Higher Dimensional Models

Theorem (Higher-Dimensional UAT for GEBLNet)

Let G be the unitary group $U(M)$. Under the same assumptions on the nonlinearity, GEBLNet can approximate arbitrarily well any square-integrable function $f \in L^2(G^K)$ such that

$$f(g_1, \ldots, g_K) = f(hg_1h^{-1}, \ldots, hg_Kh^{-1}), \quad \forall h \in G.$$

Conclusion

Our Model

GEBLNet: a gauge-equivariant neural network for predicting Chern numbers of multiband topological insulators.

Key contributions

- *Theory:* universal-approximation theorem: a sufficiently wide GEBLNet can represent *any* gauge-invariant function (incl. Chern number).
- *Practice:* high accuracy up to $N = 7$ bands.
- *Architecture:* introduced **TrNorm** layer; removes trace explosion and enables learning from topologically trivial data alone.
- *Beyond 2D:* extended to 4D grids; MAE ≈ 0.25 on the second Chern number.

Limitations and Future Work

Current gaps

- 4D discretization is approximate, not strictly integer-valued.
- Architecture explored is plain GEBL stacks; no residuals, recurrence, or attention.
- Generalization to other Lie groups untested.

Next steps

- Exact, gauge-invariant discretisations for higher Chern classes.
- Deeper or transformer-style equivariant blocks for greater expressivity.
- Broader benchmarks: other symmetry groups, experimental data.

Thank you!